Chapter 5

Maps: Calculation

In this chapter we discuss the necessary tools for the computation of transfer maps or flows of particle optical systems that relate final coordinates to initial coordinates and parameters via

\[ \tilde{z}_f = \mathcal{M}(\tilde{z}_i, \delta). \]  

(5.1)

Because the dynamics in these systems can generally be classified as being weakly nonlinear, such map methods usually rely on Taylor expansion representations of the map, assuming that this is possible. The first major code to employ such methods to second order was TRANSPORT ((Brown, Belbeoch, and Bounin 1964); (Brown 1982) (1979a), (1982)); later the methods were extended to third order in the codes TRIO (Matsuo and Matsuda 1976) and the related GIOS (Wollnik, Hartmann, and Berz 1988) and also in new versions of TRANSPORT (Carey 1992). The Lie algebraic methods developed by Dragt and coworkers (Dragt and Finn 1976; Dragt 1982) were used for the third-order code MARYLIE (Dragt, Healy, Neri, and Ryne 1985). Using custom-made formula manipulators (Berz and Wollnik 1987), an extension to fifth order was possible (Berz, Hofmann, and Wollnik 1987).

All of the previous methods are based on finding analytical representations of formulas for aberrations of a select list of elements, which inevitably makes the use of these methods complicated for high-order or very complicated fields. The differential algebraic methods introduced in Chapter 2 that are based on transforming the three key function space operations of addition, multiplication, and differentiation, to a suitable space of equivalence classes, can circumvent this difficulty. They can be used to construct algorithms that allow the computation of maps to arbitrary orders, including parameter dependence, and as discussed in Chapter 4, they can be used in principle arbitrary fields. These methods were implemented in the code COSY INFINITY (Berz 1992b), (1992b, 1993a, 1993b)) as well as in a number of other recent codes (Yan 1993; Yan and Yan 1990; van Zeijts 1993; van Zeijts and Neri 1993; Michelotti 1990; Davis, Douglas, Pusch, and Lee-Whiting, and Lee-Whiting 1993).

In this chapter, we first derive the equations of motion in particle optical coordinates using various canonical transformation tools of Hamiltonian mechanics.
and also derive equations of motion for other quantities. Then we present various differential algebra (DA)-based approaches for the determination of maps for specific cases.

5.1 The Particle Optical Equations of Motion

In this section, we will derive the equations of motion of a particle in an electromagnetic field in the so-called curvilinear coordinates. For the purposes of this section, we will neglect radiation effects as well as any influence of the spin on the orbit motion, but it will be clear from the context how to include their treatment if so desired. The curvilinear coordinates are measured in a moving right-handed coordinate system that has one of its axes attached and parallel to a given reference curve in space; furthermore, usually the time is replaced as the independent variable by the arc length along the given reference curve.

While the transformation to curvilinear coordinates seems to complicate the description of the motion, it has several advantages. First, if the chosen reference curve in space is itself a valid orbit, then the resulting transfer map will be origin preserving because the origin corresponds to the reference curve. This then opens the door to the use of perturbative techniques for the analysis of the motion in order to study how small deviations from the reference curve propagate. In particular, if the system of interest is repetitive and the reference curve is closed, then the origin will be a fixed point of the motion; perturbative techniques around fixed points can be employed to study the one-turn transfer map, which here corresponds to the Poincaré map of the motion.

Second, the method is also very practical in the sense that beams are usually rather small in size, while they often cover large territory. Therefore, it is more convenient to describe them in a local coordinate system following a reference particle instead of in a Cartesian coordinate system attached to the laboratory. Expressing the motion in terms of value of the transfer map at a given arc length very directly corresponds to the measurements by detectors, which usually determine particle coordinates at a fixed plane around the system instead of at a given time. Also, expressing the motion in terms of the arc length as an independent variable directly provides a natural scale since it is more natural to measure in meters along the system instead of in nano- or microseconds.

The following sections describe in detail the derivation of the motion in curvilinear coordinates. We will study the transformations of Maxwell’s equations and the resulting fields and their potentials to the new coordinates, and then we derive the explicit forms of the Lagrangian and Hamiltonian with time as the independent variable. Finally, a special transformation on Hamiltonians is applied that replaces time as the independent variable by the arc length, while maintaining the Hamiltonian structure of the motion.
5.1.1 Curvilinear Coordinates

Let \( \{\vec{e}_1, \vec{e}_2, \vec{e}_3\} \) denote a Dreibein, a right-handed set of fixed orthonormal basis vectors, which defines the so-called Cartesian coordinate systems. For any point in space, let \((x_1, x_2, x_3)\) denote its Cartesian coordinates. In order to introduce the curvilinear coordinates, let \( \vec{R}(s) \) be an infinitely often differentiable curve parameterized in terms of its arc length \( s \), the so-called reference curve (Fig. 5.1). For each value of \( s \), let the vector \( \vec{e}_x \) be parallel to the reference curve, i.e.,

\[
\vec{e}_x(s) = \frac{d\vec{R}}{ds}.
\]  

We now choose the infinitely often differentiable vectors \( \vec{e}_x(s) \) and \( \vec{e}_y(s) \) such that for any value of \( s \), the three vectors \( \{\vec{e}_x, \vec{e}_y, \vec{e}_y\} \) form another Dreibein, a right-handed orthonormal system. For notational simplicity, in the following we also sometimes denote the curvilinear basis vectors \( \{\vec{e}_x, \vec{e}_x, \vec{e}_y\} \) by \( \{\vec{e}_1, \vec{e}_2, \vec{e}_3\} \).

Apparently, for a given curve \( \vec{R}(s) \) there are a variety of choices for \( \vec{e}_x(s) \) and \( \vec{e}_y(s) \) that result in valid Dreibeins since \( \vec{e}_x(s) \) and \( \vec{e}_y(s) \) can be rotated around \( \vec{e}_x \). A specific choice is often made such that additional requirements are satisfied; for example, if \( \vec{R}(s) \) is never parallel to the vertical Cartesian coordinate \( \vec{e}_3 \), one may demand that \( \vec{e}_x(s) \) always lie in the horizontal plane spanned by \( \vec{e}_1 \) and \( \vec{e}_2 \).

The functions \( \vec{R}(s) \), \( \vec{e}_x(s) \), and \( \vec{e}_y(s) \) describe the so-called curvilinear coordinate system, in which a position is described in terms of \( s \), \( x \), and \( y \) via

\[
\vec{r} = \vec{R}(s) + x \vec{e}_x + y \vec{e}_y.
\]  

Apparently, the position \( \vec{r} \) in Cartesian coordinates is uniquely determined for any choice of \((s, x, y)\). The converse, however, is not generally true: A point with given Cartesian coordinates \( \vec{r} \) may lie in several different planes that are perpendicular to \( \vec{R}(s) \), as shown in Fig. 5.2.
The situation can be remedied if the curvature $\kappa(s)$ of the reference curve $\vec{R}(s)$ never grows beyond a threshold, i.e., if

$$r_1 = \frac{1}{\max_s |\kappa(s)|}$$

is finite. As Fig. 5.3 illustrates, if in this case we restrict ourselves to the inside of a tube of radius $r_1$ around $\vec{R}(s)$, for any vector within the tube, there is always one and only one set of coordinates $(s, x, y)$ describing the point $\vec{r}$.

Let us now study the transformation matrix from the Cartesian basis $\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ to the local basis of the curvilinear system $\{\vec{e}_x, \vec{e}_y, \vec{e}_z\} = \{\vec{e}_1^x, \vec{e}_2^y, \vec{e}_3^z\}$. The transformation between these basis vectors and the old ones is described by the matrix $\hat{O}(s)$, which has the form

$$\hat{O}(s) = \begin{pmatrix} \vec{e}_x(s) & \vec{e}_y(s) & \vec{e}_z(s) \end{pmatrix} = \begin{pmatrix} (\vec{e}_x \cdot \vec{e}_1) & (\vec{e}_x \cdot \vec{e}_2) & (\vec{e}_x \cdot \vec{e}_3) \\ (\vec{e}_y \cdot \vec{e}_1) & (\vec{e}_y \cdot \vec{e}_2) & (\vec{e}_y \cdot \vec{e}_3) \\ (\vec{e}_z \cdot \vec{e}_1) & (\vec{e}_z \cdot \vec{e}_2) & (\vec{e}_z \cdot \vec{e}_3) \end{pmatrix}.

(5.5)
Because the system \( \{ \vec{e}_x', \vec{e}_y', \vec{e}_z' \} \) is orthonormal, so is \( \hat{O}(s) \), and hence it satisfies
\[
\hat{O}(s) \cdot \hat{O}(s)^t = \hat{I} \quad \text{and} \quad \hat{O}(s)^t \cdot \hat{O}(s) = \hat{I}.
\]
(5.6)

Since both the old and the new bases have the same handedness, we also have
\[
\det \left( \hat{O}(s) \right) = 1,
\]
(5.7)
and hence, altogether, \( \hat{O}(s) \) belongs to the group \( SO(3) \). It must be remembered that elements of \( SO(3) \) preserve cross products, i.e., for \( \hat{O} \in SO(3) \) and any vectors \( \vec{a}, \vec{b} \), we have
\[
(\hat{O} \vec{a}) \times (\hat{O} \vec{b}) = \hat{O}(\vec{a} \times \vec{b}).
\]
(5.8)

One way to see this is to study the requirement of orthonormality on the matrix elements of \( \hat{O} \). The elements of the matrix \( \hat{O} \) describe the coordinates of the new parameter-dependent basis vectors in terms of the original Cartesian basis; explicitly, we have
\[
[e_x]_k = O_{k1}, \quad [e_y]_k = O_{k2}, \quad [e_z]_k = O_{k3}.
\]
(5.9)

The demand of the right-handedness then reads
\[
\vec{e}_i'^C \times \vec{e}_m'^C = \sum_{n=1}^{3} \epsilon_{lmn} \vec{e}_n'^C,
\]
where \( \epsilon_{ijk} \) is the common totally antisymmetric tensor of rank three defined as
\[
\epsilon_{ijk} = \begin{cases} 
1 & \text{for } (i, j, k) = (1, 2, 3) \text{ and any cyclic permutation thereof} \\
-1 & \text{for other permutations of } (1, 2, 3) \\
0 & \text{for two or more equal indices}
\end{cases}
\]
and reduces to a condition on the elements of the matrix \( \hat{O} \),
\[
\sum_{i,j=1}^{3} \epsilon_{ijk} O_{ij} O_{jm} = \sum_{n=1}^{3} \epsilon_{mnp} O_{kn}.
\]
(5.10)

It must be remembered that the symbol \( \epsilon_{ijk} \) is very useful for the calculation of vector cross products; for vectors \( \vec{a} \) and \( \vec{b} \), we have
\[
[\vec{a} \times \vec{b}]_k = \sum_{i,j=1}^{3} \epsilon_{ijk} a_i b_j.
\]
Using the condition in Eq. (5.10), we readily obtain Eq. (5.8).

For the following discussion, it is useful to study how the transformation matrix \( \hat{O} \) changes with \( s \). Differentiating Eq. (5.6) with respect to the parameter \( s \), we have

\[
0 = \frac{d}{ds}(\hat{O}^t \cdot \hat{O}) = \frac{d\hat{O}^t}{ds}\hat{O} + \hat{O}^t \frac{d\hat{O}}{ds} = \left( \hat{O}^t \frac{d\hat{O}}{ds} \right)^t + \hat{O}^t \frac{d\hat{O}}{ds}.
\]

Therefore, the matrix \( \hat{T} = \hat{O}^t \cdot \frac{d\hat{O}}{ds} \) is antisymmetric; we describe it in terms of its three free elements via

\[
\hat{O}^t \cdot \frac{d\hat{O}}{ds} = \hat{T} = \begin{pmatrix}
0 & -\tau_3 & \tau_2 \\
\tau_3 & 0 & -\tau_1 \\
-\tau_2 & \tau_1 & 0
\end{pmatrix}.
\]

We group the three elements into the vector \( \vec{\tau} \), which has the form

\[
\vec{\tau} = \begin{pmatrix}
\tau_1 \\
\tau_2 \\
\tau_3
\end{pmatrix}.
\]

We observe that for any vector \( \vec{a} \), we then have the relation

\[
\hat{T} \cdot \vec{a} = \vec{\tau} \times \vec{a}.
\]

The components of the vector \( \vec{\tau} \), and hence the elements of the matrix \( \hat{T} \), can be computed as

\[
\begin{align*}
\tau_1 &= \vec{e}_y \cdot \frac{d\vec{e}_x}{ds} = -\vec{e}_x \cdot \frac{d\vec{e}_y}{ds} \\
\tau_2 &= \vec{e}_s \cdot \frac{d\vec{e}_y}{ds} = -\vec{e}_y \cdot \frac{d\vec{e}_s}{ds} \\
\tau_3 &= \vec{e}_s \cdot \frac{d\vec{e}_x}{ds} = -\vec{e}_x \cdot \frac{d\vec{e}_s}{ds}
\end{align*}
\]

These relationships give some practical meaning to the components of the vector \( \vec{\tau} \): Apparently, \( \tau_1 \) describes the current rate of rotation of the Dreibein around the reference curve \( \vec{R}(s) \); \( \tau_2 \) describes the current amount of curvature of \( \vec{R}(s) \) in the plane spanned by \( \vec{e}_y \) and \( \vec{e}_s \); and \( \tau_3 \) similarly describes the curvature of \( \vec{R}(s) \) in the plane spanned by \( \vec{e}_x \) and \( \vec{e}_s \). In mathematical terms, because of

\[
\frac{d\vec{e}_s}{ds} = 0, \quad \frac{d\vec{e}_x}{ds} = 0, \quad \frac{d\vec{e}_y}{ds} = 0,
\]

(5.14)
we have

\[
\frac{d\vec{e}_s}{ds} = \tau_3 \vec{e}_x - \tau_2 \vec{e}_y
\]
\[
\frac{d\vec{e}_x}{ds} = -\tau_3 \vec{e}_s + \tau_1 \vec{e}_y
\]
\[
\frac{d\vec{e}_y}{ds} = \tau_2 \vec{e}_s - \tau_1 \vec{e}_x,
\]

(5.15)

as successive multiplication with \(\vec{e}_s\), \(\vec{e}_x\), and \(\vec{e}_y\) and comparison with Eq. (5.13) reveals.

As the first step in the transformation of the Maxwell’s equations and the equations of motion to the curvilinear coordinates, it is necessary to study the form of common differential operators in the new coordinates. From Eq. (5.9), which has the form

\[
\vec{r} = \sum_{k=1}^{3} x_k \vec{e}_k = \sum_{k=1}^{3} \left\{ \vec{R} \cdot \vec{e}_k + xO_{k2} + yO_{k3} \right\} \vec{e}_k,
\]

we see that the Cartesian components of \(\vec{r}\) are

\[
x_k = \vec{R} \cdot \vec{e}_k + xO_{k2} + yO_{k3} \quad \text{for } k = 1, 2, 3.
\]

(5.16)

Through extended calculation, given in detail in (Berz, Makino, and Wan 1999), all common differential operators can be expressed in terms of curvilinear coordinates.

The final differential quantity we want to express in terms of curvilinear coordinates is the velocity vector \(\vec{v}\). It is expressed as

\[
\vec{v} = v_1 \vec{e}_1 + v_2 \vec{e}_2 + v_3 \vec{e}_3 = v_s \vec{e}_s + v_x \vec{e}_x + v_y \vec{e}_y.
\]

We define

\[
\vec{v}^C = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}, \quad \vec{v}^C = \begin{pmatrix} v_s \\ v_x \\ v_y \end{pmatrix},
\]

and we have \(\vec{v}^C = \vec{O} \cdot \vec{v}^C\). To determine the velocity expressed in curvilinear coordinates, we differentiate the position vector \(\vec{r}\) with respect to time \(t\); from
Eq. (5.16), we have

\[
\dot{\sigma}^I = \frac{d\vec{r}}{dt} = \sum_{k=1}^{3} \frac{d}{dt} \left( \vec{R} \cdot \vec{e}_k + xO_{k2} + yO_{k3} \right) \vec{e}_k
\]

\[
= \sum_{k=1}^{3} \left\{ O_{k1} \dot{s} + O_{k2} \dot{x} + O_{k3} \dot{y} + \dot{s} \frac{dO_{k2}}{ds} x + \dot{s} \frac{dO_{k3}}{ds} y \right\} \vec{e}_k
\]

\[
= \hat{O} \cdot \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} + \dot{s} \frac{d\hat{O}}{ds} \cdot \begin{pmatrix} 0 \\ x \end{pmatrix} = \hat{O} \cdot \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} + \dot{s} \hat{O}^t \cdot \frac{d\hat{O}}{ds} \cdot \begin{pmatrix} 0 \\ x \end{pmatrix}
\]

\[
= \hat{O} \cdot \left\{ \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} + \dot{s} \hat{T} \cdot \begin{pmatrix} 0 \\ x \end{pmatrix} \right\} = \hat{O} \cdot \begin{pmatrix} \dot{x} (1 - \tau_3 x + \tau_2 y) \\ \dot{y} - \tau_1 y \end{pmatrix},
\]

where Eq. (5.2) is used from the first line to the second line.

For later convenience, it is advantageous to introduce the abbreviation

\[
\alpha = 1 - \tau_3 x + \tau_2 y.
\]

We note that for \( x \) and \( y \) sufficiently close to zero, \( \alpha \) does not vanish and is positive. Hence, besides the restriction for the motion to be inside a tube of radius \( r_1 \) imposed by the need for uniqueness of the transformation to curvilinear coordinates in Eq. (5.4), there is another condition; defining

\[
r_2 = \frac{1}{2} \min_s \left( \frac{1}{r_3}, \frac{1}{r_2} \right).
\]

If we restrict \( x, y \) to satisfy \( |x|, |y| < r_2 \), the quantity \( \alpha \) never vanishes.

Utilizing \( \tilde{\sigma}^I = \hat{O} \cdot \tilde{\sigma}^C \), we conclude that the velocity expressed in terms of curvilinear coordinates is given by

\[
\tilde{\sigma}^C = \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} \dot{x} (1 - \tau_3 x + \tau_2 y) \\ \dot{y} - \tau_1 y \end{pmatrix} = \begin{pmatrix} \delta \alpha \\ \hat{\tau}_1 y + \hat{\tau}_1 x \end{pmatrix}.
\]

For future reference, we note that because of the orthonormality of \( \hat{O} \), we also have the following relationships:

\[
\tilde{\sigma}^2 = \tilde{\sigma}^I \cdot \tilde{\sigma}^I = \tilde{\sigma}^C \cdot \tilde{\sigma}^C
\]

\[
\tilde{\sigma}^I \cdot \tilde{A}^d = \tilde{\sigma}^C \cdot \tilde{A}^C.
\]
5.1.2 The Lagrangian and Lagrange’s Equations in Curvilinear Coordinates

Now we are ready to develop Lagrangian and Hamiltonian methods in curvilinear coordinates. Following the transformation properties of Lagrangians, it is conceptually directly possible, albeit practically somewhat involved, to obtain the Lagrangian in curvilinear coordinates. To this end, we merely have to take the Lagrangian of a charged particle in an electromagnetic field in the Cartesian system,

\[ L(x, x_2, x_3; \dot{x}_1, \dot{x}_2, \dot{x}_3; t) = -mc^2 \sqrt{1 - \frac{v^2}{c^2}} - e\Phi + e\vec{v} \cdot \vec{A}, \]

and express all Cartesian quantities in terms of the curvilinear quantities. In this respect, it is very convenient that the scalar product of the velocity with itself and with \( \vec{v} \) is the same in the Cartesian and curvilinear systems, according to Eqs. (5.20) and (5.21). Therefore, the Lagrangian in the curvilinear system is obtained completely straightforwardly as

\[ L(s, x, y; \dot{s}, \dot{x}, \dot{y}; t) = -mc^2 \sqrt{1 - \frac{v^{\prime 2}}{c^2}} - e\Phi + e\vec{v}^{\prime} \cdot \vec{A}^{\prime}, \quad (5.22) \]

where

\[ v^{\prime 2} = v_s^2 + v_x^2 + v_y^2 \quad \text{and} \quad \vec{v}^{\prime} \cdot \vec{A}^{\prime} = v_s A_x + v_x A_x + v_y A_y. \]

Here, \( \Phi \) and \( \vec{A}^{\prime} \) are dependent on the position, i.e., \( \{s, x, y\} \), and the time \( t \). The quantities \( \ddot{O}, \ddot{T} \), and hence \( \tau_1, \tau_2, \tau_3 \) used in Eq. (5.23) are dependent on \( s \).

The derivatives of \( v_s, v_x, v_y \) with respect to \( s, x, y, \dot{s}, \dot{x}, \dot{y} \) are useful in order to determine the explicit form of Lagrange’s equations:

\[
\begin{align*}
\frac{\partial v_s}{\partial s} &= \alpha, & \frac{\partial v_s}{\partial \dot{s}} &= 0, & \frac{\partial v_s}{\partial \dot{\dot{s}}} &= 0, \\
\frac{\partial v_x}{\partial s} &= -\tau_1 y, & \frac{\partial v_x}{\partial \dot{s}} &= 1, & \frac{\partial v_x}{\partial \dot{\dot{s}}} &= 0, \\
\frac{\partial v_y}{\partial s} &= \tau_1 x, & \frac{\partial v_y}{\partial \dot{s}} &= 0, & \frac{\partial v_y}{\partial \dot{\dot{s}}} &= 1, \\
\frac{\partial v_s}{\partial \dot{s}} &= \dot{s} \left( -\frac{d\tau_3}{ds} + \frac{d\tau_2}{ds} \right), & \frac{\partial v_x}{\partial \dot{s}} &= -\dot{s} \tau_3, & \frac{\partial v_x}{\partial \dot{\dot{s}}} &= -\dot{s} \tau_2, \\
\frac{\partial v_y}{\partial \dot{s}} &= -\dot{s} \frac{d\tau_1}{ds} \dot{y}, & \frac{\partial v_y}{\partial \dot{\dot{s}}} &= \ddot{s} \tau_1, & \frac{\partial v_y}{\partial \dot{\dot{s}}} &= -\dot{s} \tau_1, \\
\frac{\partial v_x}{\partial \dot{\dot{s}}} &= \dot{s} \frac{d\tau_1}{ds} x, & \frac{\partial v_x}{\partial \dot{\dot{s}}} &= \ddot{s} \tau_1, & \frac{\partial v_y}{\partial \dot{\dot{s}}} &= 0.
\end{align*}
\]

(5.23)

The Lagrange equation for \( x \) is derived as follows. Using the derivatives of
\(v_s, v_x, v_y\) in Eq. (5.23), we have

\[
\frac{\partial v^2}{\partial x} = 2v_x \frac{\partial v_s}{\partial x} + 2v_y \frac{\partial v_x}{\partial x} + 2v_y \frac{\partial v_y}{\partial x} = 2v_x
\]

\[
\frac{\partial (v^C \cdot \bar{A}^C)}{\partial x} = A_x \frac{\partial v_x}{\partial x} + A_x \frac{\partial v_x}{\partial x} + A_y \frac{\partial v_y}{\partial x} = A_x
\]

\[
\frac{\partial v^2}{\partial x} = 2v_x \frac{\partial v_s}{\partial x} + 2v_y \frac{\partial v_x}{\partial x} + 2v_y \frac{\partial v_y}{\partial x} = -2\dot{s} (\tau_3 v_x - \tau_1 v_y) = -2\dot{s} [\vec{r} \times \vec{v}^C]_2.
\]

Altogether, we have

\[
\frac{\partial L}{\partial x} = \frac{m}{\sqrt{1 - v^2/c^2}} v_x + e A_x = p_x + e A_x,
\]

where \(\vec{p}^d = m\vec{v}^d/\sqrt{1 - v^2/c^2}\) and correspondingly \(\vec{p}^C = m\vec{v}^C/\sqrt{1 - v^2/c^2}\) was used. We also have

\[
\frac{\partial L}{\partial x} = -\frac{m}{\sqrt{1 - v^2/c^2}} \dot{s} [\vec{r} \times \vec{v}^C]_2 - e \frac{\partial}{\partial x} (\Phi - \vec{v}^C \cdot \bar{A}^C)
\]

\[
= -\dot{s} [\vec{r} \times \vec{p}^C]_2 - e \frac{\partial}{\partial x} (\Phi - \vec{v}^C \cdot \bar{A}^C).
\]

Thus, the Lagrange equation for \(x\) is

\[
\frac{dp_x}{dt} + \dot{s} [\vec{r} \times \vec{p}^C]_2 = e \left[ -\frac{dA_x}{dt} - \frac{\partial}{\partial x} (\Phi - \vec{v}^C \cdot \bar{A}^C) \right].
\]

The Lagrange equation for \(y\) is derived in the same way, and it is

\[
\frac{dp_y}{dt} + \dot{s} [\vec{r} \times \vec{p}^C]_3 = -\frac{dA_y}{dt} - \frac{\partial}{\partial y} (\Phi - \vec{v}^C \cdot \bar{A}^C).
\]

It is more complicated to derive the Lagrange equation for \(s\). Using the derivatives of \(v_s, v_x, v_y\) in Eq. (5.23), we obtain

\[
\frac{\partial v^2}{\partial s} = 2v_x \alpha - 2v_x \tau_1 y + 2v_y \tau_1 x
\]

\[
\frac{\partial (v^C \cdot \bar{A}^C)}{\partial s} = A_s \alpha - A_x \tau_1 y + A_y \tau_1 x
\]

\[
\frac{\partial v^2}{\partial s} = 2v_x \dot{s} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) - 2v_x \dot{s} \frac{d\tau_1}{ds} y + 2v_y \dot{s} \frac{d\tau_1}{ds} x
\]
Thus, the Lagrange equation for \( s \) is

\[
\frac{d}{dt}(p_s x - p_x \tau_1 y + p_y \tau_1 x) + \dot{s} x \left[ \frac{d\tau}{ds} \times \dot{p}^C \right]_2 + \dot{s} y \left[ \frac{d\tau}{ds} \times \dot{p}^C \right]_3 = e \left[ \frac{d}{ds}(A_s \alpha - A_x \tau_1 y + A_y \tau_1 x) - \frac{\partial}{\partial s}(\Phi - \dot{C} \cdot \dot{C}) \right].
\]

(5.28)

The left-hand side is modified as follows

\[
\alpha \left( \frac{dp_x}{dt} - \tau_1 y \frac{dp_x}{dt} + \tau_1 x \frac{dp_y}{dt} + \tau_2 \frac{dp_z}{dt} \right) + p_x \left( -s \frac{d\tau_3}{ds} x + \dot{s} \frac{d\tau_3}{ds} y \right) - p_x \tau_1 \dot{y} + p_y \tau_1 \dot{x}
\]

\[
+ \dot{s} x \left[ \frac{d\tau}{ds} \times \dot{p}^C \right]_2 + \dot{s} y \left[ \frac{d\tau}{ds} \times \dot{p}^C \right]_3
\]

\[
= \alpha \left( \frac{dp_x}{dt} + s[\tau \times \dot{p}^C]_1 \right) - \tau_1 y \left( \frac{dp_x}{dt} + s[\tau \times \dot{p}^C]_2 \right)
\]

\[
+ \tau_1 x \left( \frac{dp_y}{dt} + s[\tau \times \dot{p}^C]_3 \right) - v_x [\tau \times \dot{p}^C]_1 - v_y [\tau \times \dot{p}^C]_2 - v_y [\tau \times \dot{p}^C]_3
\]

\[
= \alpha \left( \frac{dp_x}{dt} + s[\tau \times \dot{p}^C]_1 \right) - \tau_1 y \left( \frac{dp_x}{dt} + s[\tau \times \dot{p}^C]_2 \right)
\]
where Eq. (5.19) is used from the second step to the third step, and

\[ v_x[\pi \times \vec{p}^C]_1 + v_y[\pi \times \vec{p}^C]_2 + v_y[\pi \times \vec{p}^C]_3 = \vec{v}^C \cdot (\vec{r} \times \vec{p}^C) = 0 \]

is used in the last step. Therefore, the Lagrange equation for \( s \) simplifies to

\[
\alpha \left( \frac{dp_x}{dt} + \dot{s}[\pi \times \vec{p}^C]_1 \right) - \tau_1 y \left( \frac{dp_y}{dt} + \dot{s}[\pi \times \vec{p}^C]_2 \right) + \tau_1 x \left( \frac{dp_y}{dt} + \dot{s}[\pi \times \vec{p}^C]_3 \right) = e \left[ -\alpha \frac{dA_x}{dt} + \tau_1 y \frac{dA_x}{dt} - \tau_1 x \frac{dA_y}{dt} + A_s \frac{d}{dt}(\tau_3 x - \tau_2 y) \right.
\]

\[
+ A_x \frac{d}{dt}(\tau_1 y) + A_y \frac{d}{dt}(\tau_1 x) - \frac{\partial}{\partial s}(\Phi - \vec{v}^C \cdot \vec{A}^C) \right].
\]

The equations for \( x \) and \( y \) (Eqs. 5.25 and 5.26) can be used to simplify the previous equation. Doing this, we obtain

\[
\alpha \left( \frac{dp_s}{dt} + \dot{s}[\pi \times \vec{p}^C]_1 \right) = e \left[ -\alpha \frac{dA_s}{dt} - \left( \frac{\partial}{\partial s} + \tau_1 y \frac{\partial}{\partial x} - \tau_1 x \frac{\partial}{\partial y} \right) (\Phi - \vec{v}^C \cdot \vec{A}^C) \right.
\]

\[
+ A_s \frac{d}{dt}(\tau_3 x - \tau_2 y) + A_x \frac{d}{dt}(\tau_1 y) + A_y \frac{d}{dt}(\tau_1 x) \right],
\]

and with the requirement that \( x \) and \( y \) are small enough such that \( \alpha = 1 - \tau_3 x + \tau_2 y > 0 \), the equation can be written as

\[
\frac{dp_s}{dt} + \dot{s}[\pi \times \vec{p}^C]_1 = e \left[ -\frac{dA_s}{dt} - \frac{1}{\alpha} \left( \frac{\partial}{\partial s} + \tau_1 y \frac{\partial}{\partial x} - \tau_1 x \frac{\partial}{\partial y} \right) (\Phi - \vec{v}^C \cdot \vec{A}^C) \right.
\]

\[
+ \frac{1}{\alpha} \left\{ A_s \frac{d}{dt}(\tau_3 x - \tau_2 y) + A_x \frac{d}{dt}(\tau_1 y) + A_y \frac{d}{dt}(\tau_1 x) \right\} \right].
\]

Thus, the set of three Lagrange equations can be summarized as follows: It apparently agrees with Newton’s equations in curvilinear coordinates [see (Berz,
Makino, and Wan (1999)].

\[
\frac{d}{dt} \begin{pmatrix} p_s \\ p_x \\ p_y \end{pmatrix} + \dot{s} \cdot \begin{pmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \end{pmatrix} \times \begin{pmatrix} p_s \\ p_x \\ p_y \end{pmatrix} = -\frac{d}{dt} \begin{pmatrix} eA_s \\ eA_x \\ eA_y \end{pmatrix} - \frac{e}{\alpha} \cdot \begin{pmatrix} \frac{\partial}{\partial s} + \tau_1 y \frac{\partial}{\partial x} - \tau_1 x \frac{\partial}{\partial y} \\ \alpha \frac{\partial}{\partial x} \\ \alpha \frac{\partial}{\partial y} \end{pmatrix} (\hat{\Phi} - \hat{v}^C \cdot \hat{A}^C)
\]

\[
+ \frac{e}{\alpha} \left\{ A_s \frac{d}{dt}(\tau_3 x - \tau_2 y) + A_x \frac{d}{dt}(\tau_1 y) + A_y \frac{d}{dt}(\tau_1 x) \right\} \hat{e}_s. \tag{5.29}
\]

5.1.3 The Hamiltonian and Hamilton’s Equations in Curvilinear Coordinates

To obtain the Hamiltonian now is conceptually standard fare, although practically it is somewhat involved. We adopt the curvilinear coordinates \( \{s, x, y\} \) as generalized coordinates, and we denote the corresponding generalized momentum by \( \vec{p}^G = (P^G_s, P^G_x, P^G_y) \). The generalized momentum is obtained via the partials of \( L \) with respect to the generalized velocities; using Eqs. (5.24) and (5.27), we obtain

\[
P^G_s = \frac{\partial L}{\partial \dot{s}} = (p_s + e A_s)\alpha - (p_x + e A_x)\tau_1 y + (p_y + e A_y)\tau_1 x
\]

\[
P^G_x = \frac{\partial L}{\partial \dot{x}} = p_x + e A_x
\]

\[
P^G_y = \frac{\partial L}{\partial \dot{y}} = p_y + e A_y. \tag{5.30}
\]

It is worthwhile to express the mechanical momentum \( \vec{p}_{\text{mech}} \), namely \( \vec{p}^G \), in terms of the generalized momentum \( \vec{p}^G = (P^G_s, P^G_x, P^G_y) \). By combining the expressions in Eq. (5.30), we have

\[
P^G_s = (p_s + e A_s)\alpha - P^G_x\tau_1 y + P^G_y\tau_1 x,
\]

and so

\[
p_s + e A_s = \frac{1}{\alpha} \left( P^G_s + P^G_x\tau_1 y - P^G_y\tau_1 x \right),
\]
and altogether
\[ \tilde{\mathbf{p}}_{\text{Mech}} = \mathbf{p}^C = \left( \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - eA_s \right) \]

(5.31)

Squaring \( \mathbf{p}^C = \gamma m \mathbf{v}^C = m \mathbf{v}^C / \sqrt{1 - (\mathbf{v}^C)^2 / c^2} \) and reorganizing yields
\[ (\mathbf{v}^C)^2 = \frac{c^2 (\mathbf{p}^C)^2}{(\mathbf{p}^C)^2 + m^2 c^2}, \]

and because \( \mathbf{v}^C \) and \( \mathbf{p}^C \) are parallel we even have
\[ \mathbf{v}^C = \frac{c \mathbf{p}^C}{\sqrt{(\mathbf{p}^C)^2 + m^2 c^2}} \]

(5.32)

We also observe that
\[ \frac{1}{\gamma} = \sqrt{1 - (\mathbf{v}^C)^2 / c^2} = \sqrt{1 - \frac{(\mathbf{p}^C)^2}{(\mathbf{p}^C)^2 + m^2 c^2}} = \frac{m c}{\sqrt{(\mathbf{p}^C)^2 + m^2 c^2}} \]

(5.33)

The Hamiltonian in the curvilinear system \( H \) is defined from the Lagrangian \( L \) (Eq. 5.22) and the generalized momentum \( \tilde{F}^G \) (Eq. 5.30) via the Legendre transformation
\[ H = \dot{s} P_s^G + \dot{x} P_x^G + \dot{y} P_y^G - L \]

\[ = \dot{s} P_s^G + \dot{x} (P_x^G + \gamma \tau_1 y) + \dot{y} P_y^G + m^2 \sqrt{1 - \frac{\mathbf{v}^C^2}{c^2}} + e \Phi - e \mathbf{v}^C \cdot \mathbf{A}^C, \]

and the subsequent expression in terms of only \( s, x, y, P_s^G, P_x^G, P_y^G \) and \( t \), if this is possible. Using Eqs. (5.31), (5.32), and (5.33), we have from Eq. (5.19) that
\[ \dot{s} = \frac{v_s}{\alpha} = \frac{1}{m \gamma} \frac{1}{\alpha} \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - eA_s \right\}, \]

\[ \dot{x} = v_x + \dot{s} \tau_1 y \]

\[ = \frac{1}{m \gamma} \left[ P_x^G - e A_x + \frac{\tau_1 y}{\alpha} \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - eA_s \right\} \right] \]

\[ = \frac{1}{m \gamma} \frac{1}{\alpha} \left\{ \tau_1 y P_s^G + (\alpha^2 + \tau_1^2 y^2) P_x^G - \tau_1^2 x y P_y^G \right) \]

\[ \dot{y} = v_y - \dot{s} \tau_1 x \]
\[ \frac{1}{m} \frac{1}{\alpha^2} \left\{ -\tau_1 x P_s^G - \tau_1^2 x y P_x^G + \left( \alpha^2 + \tau_1^2 x^2 \right) P_y^G + e\tau_1 x \alpha A_x - e\alpha^2 A_y \right\}, \]

where we used the abbreviation \( \gamma \) from Eq. (5.33), which is in terms of the generalized coordinates and the generalized momenta

\[ \frac{1}{m\gamma} = \frac{c}{\sqrt{(P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x - \alpha e A_x)^2 \alpha^2 + (P_y^G - e A_x)^2 + (P_y^G - e A_y)^2 + m^2c^2}} \]

(5.34)

We also have

\[
\vec{v}^G \cdot \vec{A}^C = \frac{1}{m\gamma} \vec{p}^G \cdot \vec{A}^C
\]

\[
= \frac{1}{m\gamma} \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x \right) - e A_s \right\} A_s
\]

\[
+ (P_y^G - e A_x) A_x + (P_y^G - e A_y) A_y, \]

and in particular it proved possible to invert the relationships between generalized velocities and generalized momenta. Hence, the Hamiltonian \( H \) can be expressed in curvilinear coordinates, and it is given by

\[
H = \frac{1}{m\gamma} \left[ \frac{1}{\alpha^2} \left( P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x \right) P_s^G + \frac{\tau_1 y}{\alpha^2} P_s^G P_x^G + \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x \right) - e A_s \right\} \frac{\tau_1 x}{\alpha} P_x^G P_y^G \right.
\]

\[
- \frac{2\tau_1^2 xy}{\alpha^2} P_x^G P_y^G - \frac{1}{\alpha} P_s^G e A_s - \frac{\tau_1 y}{\alpha} P_x^G e A_s - P_y^G e A_x + \frac{\tau_1 x}{\alpha} P_y^G e A_s
\]

\[
- P_y^G e A_y - \frac{1}{\alpha} \left( P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x \right) e A_s + e^2 A_s^2
\]

\[
- (P_x^G - e A_x) e A_x - (P_y^G - e A_y) e A_y + m^2c^2 \right\} + e\Phi
\]

\[
= \frac{1}{m\gamma} \left[ \frac{1}{\alpha^2} \left( P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x \right) \right]^2
\]

\[
- 2 \frac{1}{\alpha} \left( P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x \right) e A_s + e^2 A_s^2
\]

\[
+ (P_x^G - e A_x)^2 + (P_y^G - e A_y)^2 + m^2c^2 \right\} + e\Phi
\]

\[
= \frac{1}{m\gamma} \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G\tau_1 y - P_y^G\tau_1 x \right) - e A_s \right\}^2
\]
Explicitly, the Hamiltonian in curvilinear coordinates is

\[ H = \sqrt{(P_x^G + P_x^G \tau_1 y - P_y^G \tau_1 x - \alpha e A_s)^2 + \alpha^2 + (P_x^G - e A_x)^2 + (P_y^G - e A_y)^2 + m^2 c^2} + e \Phi, \]

where \( \alpha = 1 - \tau_3 x + \tau_2 y \). Thus we derive Hamilton’s equations as follows.

\[
\begin{align*}
\dot{s} &= \frac{\partial H}{\partial P_s} = \frac{1}{m\gamma} \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - e A_s \right\}, \\
\dot{\tau} &= \frac{\partial H}{\partial P_x} = \frac{1}{m\gamma} \left[ \frac{\tau_1 y}{\alpha} \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - e A_s \right\} \\
&\quad + P_x^G - e A_x \right\], \\
\dot{y} &= \frac{\partial H}{\partial P_y} = \frac{1}{m\gamma} \left[ \frac{\tau_1 x}{\alpha} \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - e A_s \right\} \\
&\quad + P_y^G - e A_y \right\], \\
\dot{p}_s^G &= \frac{\partial H}{\partial s} = \frac{1}{m\gamma} \left[ - \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - e A_s \right\} \\
&\quad \cdot \left\{ \frac{1}{\alpha^2} \left( \frac{dr_{\tau_3}}{ds} - \frac{dr_{\tau_2}}{ds} \right) \left( P_x^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) \\
&\quad + \frac{1}{\alpha} \left( P_x^G \frac{dr_{\tau_1}}{ds} y - P_y^G \frac{dr_{\tau_1}}{ds} x \right) - e \frac{\partial A_s}{\partial s} \right\} \\
&\quad + e \left( P_x^G - e A_x \right) \frac{\partial A_s}{\partial s} + e \left( P_y^G - e A_y \right) \frac{\partial A_s}{\partial s} \right\} - e \frac{\partial \Phi}{\partial s}, \\
\end{align*}
\]

\[
\begin{align*}
\dot{p}_x^G &= \frac{\partial H}{\partial x} = \frac{1}{m\gamma} \left[ - \left\{ \frac{1}{\alpha} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - e A_s \right\} \\
&\quad \cdot \left\{ \frac{\tau_3}{\alpha^2} \left( P_s^G + P_x^G \tau_1 y - P_y^G \tau_1 x \right) - \frac{\tau_1}{\alpha} P_y^G - e \frac{\partial A_x}{\partial x} \right\} \\
&\quad + e \left( P_x^G - e A_x \right) \frac{\partial A_x}{\partial x} + e \left( P_y^G - e A_y \right) \frac{\partial A_y}{\partial x} \right\} - e \frac{\partial \Phi}{\partial x},
\end{align*}
\]
\[ \dot{p}_y = -\frac{\partial H}{\partial y} = \frac{1}{m} \left[ -\frac{1}{\alpha} \left( p_s^G + p_x^G \tau_1 y - p_y^G \tau_1 x \right) - e A_s \right] \]

\[ \cdot \left\{ -\frac{\tau_2}{\alpha^2} \left( p_s^G + p_x^G \tau_1 y - p_y^G \tau_1 x \right) + \frac{\tau_1}{\alpha} p_x^G - e \frac{\partial A_s}{\partial y} \right\} \]

\[ + e \left( p_x^G - e A_x \right) \frac{\partial A_x}{\partial y} + e \left( p_y^G - e A_y \right) \frac{\partial A_y}{\partial y} \right] - e \frac{\partial \Phi}{\partial y}, \quad (5.38) \]

where the abbreviation \( (Eq. \ 5.34) \) is used.

To verify the derivations, we check that Hamilton’s equations agree with previous results. It is shown easily that the first three equations agree with \( \text{Eq. (5.19)} \).

The last three equations are shown to agree with Lagrange’s equations \( (5.25), (5.26), \) and \( (5.28) \). We have from \( \text{Eq. (5.37)} \)

\[ p_x^G = -\frac{1}{\alpha} \left\{ \frac{\tau_3}{\alpha} \left( p_s^G + p_x^G \tau_1 y - p_y^G \tau_1 x \right) - \tau_1 p_y^G \right\} \]

\[ + e v_x \frac{\partial A_x}{\partial x} + e v_y \frac{\partial A_y}{\partial x} - e \frac{\partial \Phi}{\partial x} \]

\[ = -\frac{\dot{s}}{\alpha} \tau_3 \frac{p_s^G}{\alpha} - \frac{\dot{s}}{\alpha} \tau_1 \frac{\tau_3 y}{\alpha} p_x^G + \dot{s} \tau_1 \left( \frac{\tau_3 x}{\alpha} + 1 \right) p_y^G \]

\[ \left\{ \frac{\partial \Phi}{\partial x} - v_x \frac{\partial A_x}{\partial x} - v_y \frac{\partial A_y}{\partial x} \right\} . \]

Expressing the equation in terms of the mechanical momentum \( \dot{p}_x^G \) rather than the generalized momentum \( \dot{p}_x^G \) according to \( \text{Eq. (5.30)} \) and using \( \text{Eq. (5.23)} \), we have

\[ \dot{p}_x + e \frac{d A_x}{dt} = -\frac{\dot{s}}{\alpha} \left\{ (p_x + e A_x) \alpha - (p_x + e A_x) \tau_1 y + (p_y + e A_y) \tau_1 x \right\} \]

\[ - \frac{\dot{s}}{\alpha} \tau_1 \frac{\tau_3 y}{\alpha} (p_x + e A_x) + \dot{s} \tau_1 \left( \frac{\tau_3 x}{\alpha} + 1 \right) (p_y + e A_y) \]

\[ - e \frac{\partial}{\partial x} \left( \Phi - v_x A_x - v_y A_y \right) \]

\[ - e \left( A_x \frac{\partial v_x}{\partial x} + A_x \frac{\partial v_x}{\partial x} + A_y \frac{\partial v_y}{\partial x} \right) \]

\[ = -\dot{s} (\tau_3 p_s - \tau_1 p_y) - e \frac{\partial}{\partial x} (\Phi - \vec{\sigma}_C \cdot \vec{x}), \]

which is in agreement with the first Lagrange equation \( (Eq. 5.25) \). The Hamilton equation for \( y \) is similarly modified from \( (Eq. 5.38) \)

\[ \dot{p}_y^G = \frac{\dot{s}}{\alpha} \frac{\tau_2}{\alpha} p_s^G + \dot{s} \tau_1 \left( \frac{\tau_2 y}{\alpha} - 1 \right) p_x^G - \frac{\dot{s}}{\alpha} \tau_1 \frac{\tau_2 x}{\alpha} p_y^G \]
In terms of the mechanical momentum $\mathbf{p}^C$, we have

$$\dot{p}_y + e \frac{dA_y}{dt} = -s(\tau_1 p_x - \tau_2 p_s) - e \frac{\partial}{\partial y}(\Phi - \mathbf{v}^C \cdot \mathbf{A}^C),$$

and it agrees with the second Lagrange equation (Eq. 5.26). Similarly, the Hamilton equation for $s$ is modified from Eq. (5.36)

$$\dot{p}_s^G = \frac{\dot{s}}{\alpha} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) p_x^G + \left\{ \frac{\dot{s}}{\alpha} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) \tau_1 y - \dot{s} \frac{d\tau_1}{ds} y \right\} p_y^G$$

where

$$\dot{p}_s = \frac{\dot{s}}{\alpha} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) \left\{ (p_x + eA_x)\alpha - (p_x + eA_x)\tau_1 y + (p_y + eA_y)\tau_1 x \right\}$$

$$+ \left\{ \frac{\dot{s}}{\alpha} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) \tau_1 y - \dot{s} \frac{d\tau_1}{ds} y \right\} (p_x + eA_x)$$

$$+ \left\{ \frac{\dot{s}}{\alpha} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) \tau_1 x + \dot{s} \frac{d\tau_1}{ds} x \right\} (p_y + eA_y)$$

$$- e \left( \frac{\partial}{\partial s} - v_x \frac{\partial A_x}{\partial s} - v_x \frac{\partial A_x}{\partial s} - v_y \frac{\partial A_y}{\partial s} \right),$$

and reorganization leads to

$$\frac{d}{dt} (p_x + eA_x)\alpha - (p_x + eA_x)\tau_1 y + (p_y + eA_y)\tau_1 x$$

$$+ \left\{ \frac{\dot{s}}{\alpha} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) \tau_1 y - \dot{s} \frac{d\tau_1}{ds} y \right\} (p_x + eA_x)$$

$$+ \left\{ \frac{\dot{s}}{\alpha} \left( -\frac{d\tau_3}{ds} x + \frac{d\tau_2}{ds} y \right) \tau_1 x + \dot{s} \frac{d\tau_1}{ds} x \right\} (p_y + eA_y)$$

$$- e \left( \frac{\partial}{\partial s} - v_x \frac{\partial A_x}{\partial s} - v_x \frac{\partial A_x}{\partial s} - v_y \frac{\partial A_y}{\partial s} \right),$$

which agrees with the third Lagrange equation (Eq. 5.28).
5.1.4 Arc Length as an Independent Variable for the Hamiltonian

As the last step, we perform a change of the independent variable from the time $t$ to the space coordinate $s$. For such an interchange, there is a surprisingly simple procedure which merely requires viewing $t$ as a new position variable, $-H$ as the associated momentum, and $-P^G_s$ as the new Hamiltonian, and expressing the interchange in terms of the new variables, if this is possible. Then the equations are

$$
\begin{align*}
\frac{dx}{ds} &= \frac{\partial(-P^G_s)}{\partial x}, & \frac{dy}{ds} &= \frac{\partial(-P^G_s)}{\partial y}, & \frac{dt}{ds} &= \frac{\partial(-P^G_s)}{\partial (-H)}, \\
\frac{dP^G_x}{ds} &= -\frac{\partial(-P^G_s)}{\partial x}, & \frac{dP^G_y}{ds} &= -\frac{\partial(-P^G_s)}{\partial y}, & \frac{d(-H)}{ds} &= -\frac{\partial(-P^G_s)}{\partial t}.
\end{align*}
$$

To begin, let us try to express $-P^G_s$ in terms of $t, x, y, -H, P^G_x,$ and $P^G_y$. From Eq. (5.35), we obtain that

$$
\left\{ \frac{1}{\alpha} \left( P^G_x + P^G_x \tau_1 y - P^G_y \tau_1 x \right) - eA_s \right\}^2
+ (P^G_x - eA_x)^2 + (P^G_y - eA_y)^2 + m^2 c^2
= \frac{1}{c^2} (H - e\Phi)^2.
$$

Therefore,

$$
\begin{align*}
(P^G_x + P^G_x \tau_1 y - P^G_y \tau_1 x - \alpha eA_s)^2
= \alpha^2 \left\{ \frac{1}{c^2} (H - e\Phi)^2 - (P^G_x - eA_x)^2 - (P^G_y - eA_y)^2 - m^2 c^2 \right\}.
\end{align*}
$$

Considering the case that $\vec{A} = 0$ and $x$ and $y$ are small, we demand $p_x$ should be positive (and stay that way throughout); it must also be remembered that $\alpha > 0$, and hence the choice of sign is made such that

$$
P^G_s = -P^G_x \tau_1 y + P^G_y \tau_1 x + \alpha eA_s
+ \alpha \sqrt{\frac{1}{c^2} (H - e\Phi)^2 - (P^G_x - eA_x)^2 - (P^G_y - eA_y)^2 - m^2 c^2}.
$$

Thus, $-P^G_s$ and hence the new Hamiltonian $H^*$ is obtained as

$$
H^* = -P^G_s = P^G_x \tau_1 y - P^G_y \tau_1 x - \alpha eA_s
- \alpha \sqrt{\frac{1}{c^2} (H - e\Phi)^2 - (P^G_x - eA_x)^2 - (P^G_y - eA_y)^2 - m^2 c^2}.
$$
Here, for later convenience, note that

\[ \sqrt{\frac{1}{c^2}(H - e\Phi)^2 - (P_x^G - eA_x)^2 - (P_y^G - eA_y)^2 - m^2 c^2} \]

\[ = \frac{1}{\alpha} \left( P_x^G + P_y^G \tau_1 y - P_y^G \tau_1 x \right) - eA_s = p_s. \]  

(5.39)

Then, the equations of motion are

\[ \frac{dx}{ds} = \frac{\partial(-P_x^G)}{\partial P_x^G} = \tau_1 y \]

\[ + \frac{\alpha(P_x^G - eA_x)}{\sqrt{\frac{1}{c^2}(H - e\Phi)^2 - (P_x^G - eA_x)^2 - (P_y^G - eA_y)^2 - m^2 c^2}}, \]  

(5.40)

\[ \frac{dy}{ds} = \frac{\partial(-P_y^G)}{\partial P_y^G} = -\tau_1 x \]

\[ + \frac{\alpha(P_y^G - eA_y)}{\sqrt{\frac{1}{c^2}(H - e\Phi)^2 - (P_x^G - eA_x)^2 - (P_y^G - eA_y)^2 - m^2 c^2}}, \]  

(5.41)

\[ \frac{dt}{ds} = \frac{\partial(-P_x^G)}{\partial(-H)} \]

\[ = \frac{\alpha}{c^2} \frac{1}{\sqrt{\frac{1}{c^2}(H - e\Phi)^2 - (P_x^G - eA_x)^2 - (P_y^G - eA_y)^2 - m^2 c^2}}, \]  

(5.42)

\[ \frac{dP_x^G}{ds} = -\frac{\partial(-P_x^G)}{\partial x} = P_y^G \tau_1 - e\tau_3 A_s + \alpha e \frac{\partial A_s}{\partial x} \]

\[ - \tau_3 \sqrt{\frac{1}{c^2}(H - e\Phi)^2 - (P_x^G - eA_x)^2 - (P_y^G - eA_y)^2 - m^2 c^2} \]

\[ - \frac{1}{c^2} \frac{\partial\Phi}{\partial x} - (P_x^G - eA_x) \frac{\partial A_x}{\partial x} - (P_y^G - eA_y) \frac{\partial A_y}{\partial x}, \]

\[ \sqrt{\frac{1}{c^2}(H - e\Phi)^2 - (P_x^G - eA_x)^2 - (P_y^G - eA_y)^2 - m^2 c^2} \]

\[ \frac{dP_y^G}{ds} = -\frac{\partial(-P_y^G)}{\partial y} = -P_x^G \tau_1 + e\tau_2 A_s + \alpha e \frac{\partial A_s}{\partial y} \]  

(5.44)
\[
\begin{align*}
&+ \tau_2 \sqrt{\frac{1}{c^2} (H - e\Phi)^2 - (P^G_x - eA_x)^2 - (P^G_y - eA_y)^2 - m^2c^2} \\
&- \alpha e \frac{1}{c^2} \left( H - e\Phi \right) \frac{\partial \Phi}{\partial y} - \left( P^G_x - eA_x \right) \frac{\partial A_x}{\partial y} - \left( P^G_y - eA_y \right) \frac{\partial A_y}{\partial y} \right), \\
&\sqrt{\frac{1}{c^2} (H - e\Phi)^2 - (P^G_x - eA_x)^2 - (P^G_y - eA_y)^2 - m^2c^2}.
\end{align*}
\]

\[
\frac{d(-H)}{ds} = -\frac{\partial(-P^G_x)}{\partial t} = \alpha \left[ \frac{\partial A_x}{\partial t} \right] (5.45)
\]

For the sake of convenience and checking purposes, we replace \( P^G_x, P^G_y \), and \( H \) by \( \vec{p}^G \) using Eqs. (5.30) and (5.35), with the help of Eqs. (5.32) and (5.39). Then we have from Eqs. (5.40), (5.41) and (5.42)

\[
\begin{align*}
&\frac{dx}{ds} = \tau_1 y + \frac{p_x}{p_s} \\
&\frac{dy}{ds} = -\tau_1 x + \frac{p_y}{p_s} \\
&\frac{dt}{ds} = \frac{1}{p_s} \sqrt{(\vec{p}^G)^2 + m^2c^2}.
\end{align*}
\]

We have from Eq. (5.43)

\[
\frac{dp_x}{ds} + e \frac{dA_x}{ds} = (p_y + eA_y)\tau_1 - e\tau_3 A_x + \alpha e \frac{\partial A_x}{\partial x} - \tau_3 p_s \\
- \frac{e}{p_s} \left\{ \frac{\sqrt{(\vec{p}^G)^2 + m^2c^2}}{c} \frac{\partial \Phi}{\partial x} - p_x \frac{\partial A_x}{\partial x} - p_y \frac{\partial A_y}{\partial x} \right\},
\]

and organizing the expression using Eqs. (5.23), (5.19), and (5.32) we find

\[
\frac{dp_x}{ds} + \left[ \vec{\tau} \times \vec{p}^G \right]_x = e \left[ - \frac{dA_x}{ds} - \frac{1}{s} \frac{\partial}{\partial x} (\Phi - \vec{\sigma} \cdot \vec{A}^c) \right]. (5.48)
\]

In a similar way, we obtain from Eq. (5.44)

\[
\frac{dp_y}{ds} + \left[ \vec{\tau} \times \vec{p}^G \right]_y = e \left[ - \frac{dA_y}{ds} - \frac{1}{s} \frac{\partial}{\partial y} (\Phi - \vec{\sigma} \cdot \vec{A}^c) \right], (5.49)
\]
and from Eq. (5.45)
\[
\frac{dH}{ds} = \frac{1}{s} \frac{\partial}{\partial t} \left[ e(\Phi - \vec{\Phi} \cdot \vec{A'}) \right].
\]

This concludes the derivations of dynamics in curvilinear coordinates. In particular, we have succeeded in deriving the equations of motion of a particle moving in an electromagnetic field in curvilinear coordinates, with the arc length \( s \) as the independent variable. Moreover, we know that these equations of motion are Hamiltonian in nature, which has important consequences for theoretical studies.

### 5.1.5 Curvilinear Coordinates for Planar Motion

As an application of the concepts just derived, we consider a particularly important special case, namely, the situation in which the reference curve stays in the \( x_1x_2 \) plane. This so-called two-dimensional (2-D) curvilinear system occurs frequently in practice, in particular if the reference curve is an actual orbit and the fields governing the motion have a symmetry around the horizontal plane. The basis vectors in this 2-D curvilinear system can be expressed by the Cartesian basis vectors via

\[
\vec{e}_y = \vec{e}_3
\]
\[
\vec{e}_x = \cos \theta \vec{e}_1 - \sin \theta \vec{e}_2
\]
\[
\vec{e}_z = \sin \theta \vec{e}_1 + \cos \theta \vec{e}_2,
\]

where \( \theta \) depends on the arc length \( s \), and its derivative is denoted by \( h \), i.e.,
\[
h = h(s) = \frac{d\theta(s)}{ds}.
\]

From Eq. (5.9), all the elements of the matrix \( \hat{O} \) are determined as

\[
\hat{O} = \begin{pmatrix}
\cos \theta & \sin \theta & 0 \\
-\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix}.
\]

Therefore, the antisymmetric matrix \( \hat{T} \) of Eq. (5.11) has the form
\[
\hat{T} = \hat{O}^t \cdot \frac{d\hat{O}}{ds} = \begin{pmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix} \begin{pmatrix}
-\sin \theta \cdot h & \cos \theta \cdot h & 0 \\
-\cos \theta \cdot h & -\sin \theta \cdot h & 0 \\
0 & 0 & 0
\end{pmatrix} = \begin{pmatrix}
0 & h & 0 \\
-h & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\]
Thus, the elements of $\mathbf{T}$ and hence $\mathbf{r}$ are given as

$$
\mathbf{r}' = \begin{pmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -h \\ \end{pmatrix};
$$

finally, we have

$$
\alpha = 1 - \tau_3 x + \tau_2 y = 1 + hx.
$$

The velocity expressed in this system is, from Eq. (5.19),

$$
\mathbf{v}' = \begin{pmatrix} v_s \\ v_x \\ v_y \\ \end{pmatrix} = \begin{pmatrix} \dot{s}(1 + hx) \\ \dot{x} \\ \dot{y} \\ \end{pmatrix}.
$$

Thus, the equations of motion expressed in this system are

$$
\frac{d}{dt} \begin{pmatrix} p_s \\ p_x \\ p_y \end{pmatrix} + \dot{s} \begin{pmatrix} 0 \\ 0 \\ -h \end{pmatrix} \times \begin{pmatrix} p_s \\ p_x \\ p_y \end{pmatrix} = \begin{pmatrix} \frac{dp_s}{dt} + \dot{s}p_x \\ \frac{dp_x}{dt} - \dot{s}p_s \\ \frac{dp_y}{dt} \end{pmatrix}
$$

$$
= e \left[ -\frac{d}{dt} \begin{pmatrix} A_x \\ A_x \\ A_y \end{pmatrix} - \begin{pmatrix} 1 \\ \frac{1 + hx}{\dot{\tau}_3} \frac{\partial}{\partial s} \\ \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} (\Phi - \mathbf{v}' \cdot \mathbf{A}') \right. 
$$

$$
+ \begin{pmatrix} A_x d/dt(-hx) \\ \frac{1 + hx}{\dot{\tau}_3} \frac{\partial}{\partial s} \\ \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} \right].
$$

Furthermore, the equations of motion after space–time interchange in this system are, from Eqs. (5.48) and (5.49),

$$
\frac{dp_x}{ds} - hp_s = e \left[ -\frac{dA_x}{ds} - \frac{1}{\dot{s}} \frac{\partial}{\partial x} (\Phi - \mathbf{v}' \cdot \mathbf{A}') \right]
$$

$$
\frac{dp_y}{ds} = e \left[ -\frac{dA_y}{ds} - \frac{1}{\dot{s}} \frac{\partial}{\partial y} (\Phi - \mathbf{v}' \cdot \mathbf{A}') \right].
$$
Here, $E_{x,y,s}$ and $B_{x,y,s}$ are the electric and magnetic field components in the $x$, $y$, and $s$ directions, respectively.

It is customary to express the equations of motion in terms of the normalized coordinates $a = p_x/p_0$ and $b = p_y/p_0$, where $p_0$ is a reference momentum. Expressed in these coordinates, the complete equations of motion take the form

$$\frac{dx}{ds} = (1 + hx) \frac{a}{\sqrt{(p/p_0)^2 - a^2 - b^2}}$$

$$\frac{dy}{ds} = (1 + hx) \frac{b}{\sqrt{(p/p_0)^2 - a^2 - b^2}}$$

$$\frac{da}{ds} = h \cdot \sqrt{(p/p_0)^2 - a^2 - b^2} + \frac{e}{p_0} \left[ \frac{1}{s} E_x + \frac{dy}{ds} B_s - (1 + hx) B_x \right]$$

$$\frac{db}{ds} = \frac{e}{p_0} \left[ \frac{1}{s} E_y - \frac{dx}{ds} B_s + (1 + hx) B_x \right]$$

5.2 Equations of Motion for Spin

The equation for the classical spin vector $\vec{S}$ of a particle in the electromagnetic field is generally assumed to have the form of the Thomas–BMT equation (Thomas 1927; V. Bargmann and Telegdi 1959):

$$\frac{d\vec{S}}{dt} = \vec{W} \times \vec{S},$$

where the vector $\vec{W}$ is given by

$$\vec{W} = -\frac{e}{m \gamma} \left\{ \frac{(1 + \gamma G)}{(1 + \gamma)} \vec{B} - \frac{G}{m \gamma} \frac{\vec{p} \cdot \vec{B}}{m c^2} \vec{p} - \left( G + \frac{1}{1 + \gamma} \right) \frac{1}{m c^2} \vec{p} \times \vec{E} \right\}.$$

Here, $G = (g - 2)/2$ quantifies the anomalous spin factor, $\vec{p}$ is the kinetic momentum of the particle, and the time $t$ is the independent variable.

A careful analysis reveals that the above formula perhaps poses more questions than it answers, because its detailed derivation hinges on several assumptions. First, the equation should be relativistically covariant; it should reduce to the proper nonrelativistic equation in the rest frame of the particle; and it should be linear in the field. While these assumptions appear plausible, caution may already be in order because the orbital motion of the particle in the field is also
accelerated, perhaps opening the door for the requirement to treatment in general relativity. But many further assumptions are necessary, including that spin is described by a four-vector (and not connected to a tensor like the magnetic field it represents), about the maximal orders of dependencies on four-velocities, and the preservation of various products of four-vectors and tensors. For some details, refer to (Thomas 1927; V. Bargmann and Telegdi 1959; Parrott 1987; Rohrlich 1990). Some of the complexities of the arguments are illuminated when comparing the results stated in the first and second edition of (Rohrlich 1990). While Eq. (5.55) seems to agree well with experimental evidence, its deep theoretical foundations at this point appear rather unclear and worthy of further study.

If we express the motion in curvilinear coordinates \((s, x, y)\) with arc length \(s\) as an independent variable as in Eq. (5.2), the spin motion equation (Eq. 5.55) takes the form

\[
\frac{d\vec{s}}{ds} = \vec{W}^* \times \vec{s},
\]

(5.56)

where

\[
W^*_s = (1 - \tau_3 x + \tau_2 y) \frac{m_\gamma}{p_\gamma} W_z; \\
W^*_x = -\tau_2 + (1 - \tau_3 x + \tau_2 y) \frac{m_\gamma}{p_\gamma} W_x; \\
W^*_y = -\tau_3 + (1 - \tau_3 x + \tau_2 y) \frac{m_\gamma}{p_\gamma} W_y;
\]

(5.57)

Here \((W^*_s, W^*_x, W^*_y)\) are the components of the vector \(\vec{W}^*\) expressed in the new variables \((s, x, y)\), \(p_\gamma\) is the longitudinal kinetic momentum, \(\tau_3\) and \(\tau_2\) are the curvatures in the \(x\) and \(y\) directions introduced in Eq. (5.12), where \(\tau_1\) is assumed to be zero.

For further discussion, it is useful to introduce the matrix \(\vec{W} (\vec{z})\), which is made from the vector \(\vec{W}^* (\vec{z})\) via

\[
\vec{W} (\vec{z}) = \begin{pmatrix}
0 & -W^*_y & W^*_x \\
W^*_y & 0 & -W^*_z \\
-W^*_x & W^*_z & 0
\end{pmatrix}.
\]

(5.58)

Note that the matrix \(\vec{W}\) is antisymmetric and, using \(\vec{W}\), the spin equations of motion can be written as

\[
\frac{d\vec{s}}{ds} = \vec{W} \cdot \vec{s}.
\]

(5.59)

The particular form of the equation of motion (Eq. 5.56) entails that the solution always has a particular form. Because the equations of motion are linear in
the spin, the final transformation of the spin variables can be described in terms of a matrix that depends only on the orbital quantities. The orbital quantities themselves are unaffected by the spin motion, such that altogether the map has the form

\[
\begin{aligned}
&\mathcal{Z}_f = \mathcal{M}(\mathcal{Z}_i, s), \\
&\mathcal{S}_f = \mathcal{A}(\mathcal{Z}_i, s) \cdot \mathcal{S}_i.
\end{aligned}
\]  

(5.60)

The special cross product form of the spin motion imposes a restriction on the matrix \(\mathcal{A}\) in that the matrix is orthogonal with determinant \(6\), i.e., \(\mathcal{A}(\mathcal{Z})\) satisfies \(\mathcal{A}^t(\mathcal{Z}) \cdot \mathcal{A}(\mathcal{Z}) = I\) and \(\det(\mathcal{A}(\mathcal{Z})) = 1\). We will demonstrate this using similar arguments as presented in Section 1.4.7 in the proof that flows of Hamiltonian systems are symplectic. Let us consider an ODE \(\frac{d}{dt} \mathcal{r} = \mathcal{W}(t) \cdot \mathcal{r}\), where the \(n\)-dimensional matrix \(\mathcal{W}\) is antisymmetric. Since the equation is linear, so is the flow, and we have

\[
\mathcal{r}(t) = \mathcal{A}(t) \cdot \mathcal{r}_0,
\]  

(5.61)

where \(\mathcal{A}\) is the Jacobian of the flow. Define

\[
\dot{\mathcal{P}}(t) = \mathcal{A}^t(t) \cdot \mathcal{A}(t).
\]

(5.62)

Initially, \(\dot{\mathcal{P}}\) equals the identity, and so \(\dot{\mathcal{P}}(t_0) = I\). The equations of motion entail that the motion of the matrix \(\mathcal{A}\) can be described by

\[
\frac{d}{dt} \mathcal{A}(t) = \mathcal{W} \cdot \mathcal{A}(t),
\]

(5.63)

which in turn entails that

\[
\frac{d}{dt} \dot{\mathcal{P}}(t) = \frac{d}{dt} (\mathcal{A}^t(t) \cdot \mathcal{A}(t)) = \mathcal{A}^t \cdot \mathcal{W}^t \cdot \mathcal{A} + \mathcal{A}^t \cdot \mathcal{W} \cdot \mathcal{A} = 0.
\]

(5.64)

This entails that one solution of the ODE for \(\dot{\mathcal{P}}(t)\) that satisfies the necessary initial condition \(\dot{\mathcal{P}}(t_0) = I\) is

\[
\dot{\mathcal{P}}(t) = I \text{ for all } t.
\]

(5.65)

However, because of the uniqueness theorem for differential equations, this is also the only solution, and we have proved what we wanted to show. We now consider the determinant of the matrix. Because \(1 = \det(\dot{\mathcal{P}}(t)) = \det(\mathcal{A}^t(t) \cdot \mathcal{A}(t)) = \)
det(\(A(t)\))², we have det(\(M\)) = ±1. However, since \(\dot{A}\) and hence det(\(\dot{A}\)) depend continuously on time and det(\(\dot{A}\)) = 1 for \(t = t_0\), we must have that

\[
det(\dot{A}) = +1.
\] (5.66)

Therefore, \(\dot{A} \in SO(n)\), as we wanted to show.

The practical computation of the spin-orbit map can be achieved in a variety of ways. Conceptually, the simplest way is to interpret it as a motion in the nine variables consisting of orbit and spin described by the orbit equations as well as the spin equations (Eq. 5.56). In this case, the DA method allows the computation of the spin-orbit map in two conventional ways (see Section 5.4), namely, via a propagation operator for the case of the \(s\)-independent fields, such as main fields, and via integration of the equations of motion with DA, as described in Chapter 2, Section 2.3.4. However, in this simplest method, the number of independent variables increases from six to nine, which particularly in higher orders entails a substantial increase in computational and storage requirements. This severely limits the ability to perform analysis and computation of spin motion to high orders.

Instead, it is more advantageous to keep only six independent variables but to augment the differential equations for the orbit motion by the equations of the orbit-dependent spin matrix which have the form

\[
\dot{\mathcal{A}}(\mathcal{z}) = \hat{W}(\mathcal{z}) \cdot \mathcal{A}(\mathcal{z}).
\] (5.67)

If desired, the \(SO(3)\) structure of \(\mathcal{A}\) can be used to reduce the number of additional differential equations at the cost of slight subsequent computational expense. The most straightforward simplification results from the fact that since orthogonal matrices have orthogonal columns and their determinant is unity and hence the orientation of a Dreibein is preserved, it follows that the third column of the matrix \(\mathcal{A}(\mathcal{z}) = (\mathcal{A}_1(\mathcal{z}), \mathcal{A}_2(\mathcal{z}), \mathcal{A}_3(\mathcal{z}))\) can be uniquely calculated via

\[
\mathcal{A}_3(\mathcal{z}) = \mathcal{A}_1(\mathcal{z}) \times \mathcal{A}_2(\mathcal{z}).
\] (5.68)

Thus, in this scenario, only six additional differential equations without new independent variables are needed for the description of the dynamics. For the case of integrative solution of the equations of motion, which is necessary in the case of \(s\)-dependent elements, these equations can be integrated in DA with any numerical integrator.

However, for the case of main fields, the explicit avoidance of the spin variables in the previously described manner is not possible since, for reasons of computational expense, it is desirable to phrase the problem in terms of a propagator operator

\[
\begin{pmatrix}
\frac{z_f}{\mathcal{S}_f} \\
\mathcal{S}_f
\end{pmatrix} = \exp(\Delta s \cdot \mathcal{L}_f) \begin{pmatrix}
\frac{z}{\mathcal{S}} \\
\mathcal{S}
\end{pmatrix}.
\] (5.69)
Here, \( L \vec{f} = \vec{F} \cdot \vec{\nabla} \) is the nine-dimensional vector field belonging to the spin–orbit motion. In this case, the differential vector field \( L \vec{f} \) describes the entire motion including that of the spin, i.e., \( d/ds(\vec{z}, \vec{S}) = \vec{F}(\vec{z}, \vec{S}) = (\vec{f}(\vec{z}), \vec{W}^* \times \vec{S}) \). In particular, the operator \( L \vec{f} \) contains differentiation with respect to the spin variables, which requires their presence. Therefore, the original propagator is not directly applicable for the case in which the spin variables are dropped and has to be rephrased for the new choice of variables. For this purpose, we define two spaces of functions \( g(\vec{z}, \vec{S}) \) on spin–orbit phase space as follows:

\[ Z: \text{Space of functions depending only on } \vec{z} \]
\[ S: \text{Space of linear forms in } \vec{S} \text{ with coefficients in } Z \]

Then, we have for \( g \in Z \),

\[
L \vec{f} g = \left( \vec{f} \cdot \vec{\nabla}_{\vec{z}} + (\vec{W} \cdot \vec{S})^t \cdot \vec{\nabla}_{\vec{S}} \right) g = \vec{f} \cdot \vec{\nabla}_{\vec{z}} g = L \vec{f} g, \tag{5.70}
\]

and in particular, the action of \( L \vec{f} \) can be computed without using the spin variables; furthermore, since \( \vec{f} \) depends only on \( \vec{z} \), we have \( L \vec{f} g \in Z \). Similarly, we have for \( g = |a_1, a_2, a_3\rangle = \sum_{j=1}^3 a_j \cdot S_j \in S \),

\[
L \vec{f} |a_1, a_2, a_3\rangle = (\vec{f} \cdot \vec{\nabla}_{\vec{z}} + (\vec{W} \cdot \vec{S})^t \cdot \vec{\nabla}_{\vec{S}}) \left( \sum_{j=1}^3 a_j \cdot S_j \right)
\]

\[
= \sum_{j=1}^3 (\vec{f} \cdot \vec{\nabla}_{\vec{z}}) a_j \cdot S_j + \sum_{j,k=1}^3 S_j W_{kj} a_k
\]

\[
L \vec{f} a_1 + \sum_{k=1}^3 W_{k1} a_k , \quad L \vec{f} a_2 + \sum_{k=1}^3 W_{k2} a_k , \quad L \vec{f} a_3 + \sum_{k=1}^3 W_{k3} a_k \tag{5.71}
\]

and in particular, the action of \( L \vec{f} \) can be computed without using the spin variables; furthermore, \( L \vec{f} |a_1, a_2, a_3\rangle \in S \). Thus, \( Z \) and \( S \) are \textit{invariant subspaces} of the operator \( L \vec{f} \). Furthermore, the action of the nine-dimensional differential operator \( L \vec{f} \) on \( S \) is uniquely described by Eq. (5.71), which expresses it in terms of the six-dimensional differential operator \( L \vec{f} \). This allows the computation of the action of the \textit{original propagator} \( \exp(\Delta \cdot L \vec{f}) \) on the identity in \( \mathcal{R}^9 \), the result of which actually describes the total nine-dimensional map. For the top six lines of the identity, note that the components are in \( Z \), and hence the repeated application of \( L \vec{f} \) will stay in \( Z \); for the bottom three lines, those of the identity
The most straightforward methods for the determination of maps in the neighborhood of the reference trajectory through Taylor expansion are applicable where the motion under consideration is determined merely by algebraic equations. These cases include lens-based light optics, the motion in magnetic dipoles, and an approximation frequently used for high-energy accelerators based on drifts and kicks.

5.3.1 Lens Optics

Lens optics represents the special case of light optics in which the system under consideration consists of an ensemble of individual glass objects \( g_i \) with index of refraction \( n_i \), separated by drifts of length \( l_i \). It thus represents the practically and historically most important case of the general optical problem, which is described in terms of an index of refraction \( n(x, y, z) \) that is dependent on position and that affects local propagation velocity via \( v = c/n(x, y, z) \). The motion is described by Fermat’s principle, which states that the light ray between two points follows the fastest path. The general problem is described in terms of Lagrange equations with the Lagrangian

\[
L = n(x, y, z) \cdot \sqrt{1 + \left( \frac{dz}{dx} \right)^2 + \left( \frac{dy}{dx} \right)^2}.
\]  

As a consequence of Fermat’s principle, light rays follow straight paths in regions where the index of refraction is constant. On the other hand, at transitions between regions in which the index of refraction is constant, the direction of travel of the light ray changes as dictated by Snell’s Law of refraction.
The most common glass element is the lens shown in Fig. 5.4. In the most general case, the left and right surfaces of the glass lens are given by functions

\[ S_1(x, y) \text{ and } S_2(x, y), \]  

(5.74)

describing the shape of the surface relative to the so-called entrance and exit planes. Frequently, the surfaces \( S_1 \) and \( S_2 \) are spherical.

The motion of a ray is completely determined by the ray-tracing scheme, in which the ray is propagated until it hits a transition surface, then refracted following Snell’s law, then propagated to the next surface, and so on. In the case of spherical lenses, the intersection with the next surface can usually be calculated in closed form. In the case of a general surface \( S(x, y) \), the ray is usually propagated to the plane tangent to \( S \) at \((x, y) = (0,0)\). Denoting its position in this plane by \((x_r, y_r)\), its distance to the lens is given approximately by \( S(x_r, y_r) \), and the particle is propagated along a straight line by this distance. Its new positions \((x_r, y_r)\) are determined, and the method is iterated until convergence to sufficient accuracy is obtained.

To determine the map of such a glass optical system, one merely has to recognize that the ray-tracing scheme provides a functional dependence of final conditions on initial conditions and parameters, and to evaluate the entire scheme within DA utilizing Eq. (2.96).

As an example of the approach, we calculate nonlinearities of the map of the Kitt Peak telescope (Wynne 1973) up to order 13. To illustrate the effects, we plot the focal point positions of an ensemble of parallel rays of an angle of 20 minutes of arc, striking the main mirror at different positions. The results are shown in Fig. 5.5. Apparently, the telescope is designed so that fifth-order terms help compensate third-order terms. Going from fifth to seventh order then shows an increase in spot size, apparently because seventh-order terms have not been corrected. Going from seventh to thirteenth order does not result in additional effects, suggesting that for the rays selected, the device is well described by order seven.
5.3.2 The Dipole

Another case where the map of a system is uniquely determined through mere geometric relationships is the motion in a dipole magnet with a uniform magnetic field. The general shape of such a magnet, the reference trajectory, and a particle trajectory are shown in Fig. 5.6.

Analytic computation is possible, because charged particles experience a force in the plane perpendicular to the field direction, which produces circular motion in the projection on that plane, which we call the $x-s$ plane. In the direction parallel to the homogeneous field, no force is produced and the particles perform a force-free drift in that direction.

We are looking for the map which relates canonical particle optical coordinates $z_i$ in front of the magnet to the final coordinates $z_f$ behind the magnet. The initial
plane is denoted by \( s_i \) and the final plane by \( s_f \). The entrance curve of the magnet relative to the entrance plane is given by the function \( f_i(x) \) and the exit curve is described by the function \( f_f(x) \). The projected motion through the magnet can therefore be given by successively computing three separate parts of the motion:

1. motion on a line from \( s_i \) to the curve \( f_i \)
2. motion on a circle from \( f_i \) to \( f_f \)
3. motion on a line from \( f_f \) to \( s_f \).

Since the analytic solution is based on the geometry of the motion, we first have to transform from canonical coordinate \( \xi \) to geometric coordinates \( \xi' \) containing positions and slopes. After that, the trajectory can be determined analytically by straightforward geometry. Finally, the geometric coordinates \( \xi' \) have to be transformed back to the canonical notation \( \xi_p \).

As an example for the analytical calculation of high-order maps of bending magnets, we consider the aberrations of the so-called Browne–Buechner magnet. It consists of a single dipole magnet with a deflection angle of \( 90^\circ \). The entrance and exit pole faces are not tilted, but rather curved with a radius equal to the deflection radius. Therefore, the resulting dipole can be made from a simple circular magnet. The layout of a Browne–Buechner magnet is shown in Fig. 5.7.

The magnet is usually preceded and followed by equal drifts to obtain horizontal imaging, i.e., to make the final coordinates independent of initial directions in linear approximation. According to Barber’s rule, this requires the drifts to have a length equal to the deflection radius \( R \). It has been shown by basic yet elaborate geometrical arguments that this geometrical layout entails that all second-order geometric aberrations in the \( x-s \) projection vanish, which is very helpful for improving the resolution of the device (see Chapter 6, Section 6.3.1).

DA methods can now be used to obtain the high-order map of the system. To this end, we perform the various steps of the geometric calculations to determine the position of the particle as a function of the initial \((x, \alpha)\) coordinates. Similar
to the previous section, they are merely evaluated with DA following Eq. (2.96) to obtain as many high-order derivatives as desired.

Table I shows the resulting aberrations for both position and angle in the focal plane to fifth order. The calculation has been performed for a deflection radius of 1 m; since this deflection radius is the only free parameter, and obviously

TABLE I
ABERRATIONS OF UP TO ORDER FIVE OF THE BROWNE–BUECHNER MAGNET. ALL SECOND-ORDER ABERRATIONS VANISH.

| \( x_f | x_i^a a_i^b \) | \( a_f | x_i^a a_i^b \) | \( i_x \) | \( i_o \) |
|---|---|---|---|
| -1.0000000000000000 | -1.0000000000000000 | 1 | 0 |
| -0.5000000000000000 | -1.0000000000000000 | 3 | 0 |
| -2.0000000000000000 | -0.5000000000000000 | 2 | 1 |
| -3.0000000000000000 | -1.0000000000000000 | 1 | 2 |
| -2.0000000000000000 | -1.0000000000000000 | 0 | 3 |
| -0.3750000000000000 | 0.0000000000000000 | 5 | 0 |
| -2.7500000000000000 | -0.1250000000000000 | 4 | 1 |
| -8.0000000000000000 | -1.0000000000000000 | 3 | 2 |
| -12.5000000000000000 | -2.5000000000000000 | 2 | 3 |
| -10.7500000000000000 | -3.0000000000000000 | 1 | 4 |
| -4.5000000000000000 | -1.7500000000000000 | 0 | 5 |
the whole geometry scales with it, this device is representative of all Browne–Buechner magnets.

It is possible in principle to compute analytical formulas for the aberrations of higher orders by differentiating the analytical formulas relating final coordinates to initial coordinates. However, due to the complexity of the formulas, this quickly leads to cumbersome expressions. The use of DA, on the other hand, allows the calculation of higher-order aberrations as effortlessly as did the plain numeric evaluation of formulas with numbers, except for an increase of computation time and storage requirements.

To illustrate this point, we computed all aberrations of the Browne–Buechner magnet up to order 39. The results are shown in Table II, where for reasons of space, we restrict ourselves to the opening aberrations of the form \((x, a^n)\).

All aberrations of even order vanish. Furthermore, the aberrations have a tendency to be quite benign, and there is much interesting asymptotic behavior, which is also exemplified in Table II.

<table>
<thead>
<tr>
<th>(x \cdot a^n)</th>
<th>(n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

**TABLE II**

<table>
<thead>
<tr>
<th>(x \cdot a^n)</th>
<th>(n)</th>
</tr>
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<tbody>
<tr>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

**ABERRATIONS OF UP TO ORDER 39 OF THE BROWNE–BUECHNER MAGNET. FOR REASONS OF SPACE, WE LIMIT OURSELVES TO THE SO-CALLED OPENING ABERRATIONS \((x, a^n)\).**
5.3.3 Drifts and Kicks

The method of kicks and drifts is an approximation for the motion through particle optical elements that is often employed in high energy accelerators, and often yields satisfactory results. To this end, the motion through the element under consideration that is governed by the ODE $d(x, y, d, a, b, t)/dt = \vec{f}(x, y, d, a, b, t)$ is assumed to begin with a drift to the middle of the element of length $L$, followed by a kick changing only momenta and given by

$$
\Delta a = L \cdot f_a(x, y, d, a, b, t) \\
\Delta b = L \cdot f_b(x, y, d, a, b, t),
$$

(5.75)

and finally conclude with another drift to the end of the element. The accuracy of this approximation depends on the actual amount of curvature of the orbit; if each element affects the motion by only a very small amount, then the force on the particle is reasonably approximated by the force experienced by a particle merely following a straight line. By evaluating the force in the middle of the trajectory, any variation over the course of the straight line is averaged out to some degree.

Apparently, the simple kick model described by Eq. (5.75) leads to a relationship of final coordinates in terms of initial coordinates by a sequence of elementary operations and functions, and, via Eq. (2.96), allows the computation of maps of the approximated motion to any order of interest.

5.4 Maps Determined by Differential Equations

For maps determined by differential equations, the DA methods introduced in Chapter 2 allow the determination of high-order nonlinearities in a convenient and rather straightforward way. DA methods can be used to construct algorithms that allow the computation of maps to arbitrary orders, including parameter dependence and arbitrary fields. In this section we outline various approaches to this goal, based both on conventional ODE solvers and on new algorithms intimately connected to the differential algebraic framework.

5.4.1 Differentiating ODE Solvers

Intuitively, the most direct method for obtaining Taylor expansions for the flow of an ODE is to recognize that a numerical ODE solver describes a functional dependency between initial conditions and final conditions. Thus, by replacing all arithmetic operations in it by the corresponding ones in the differential algebra $\mathbb{K}[D]$, we readily obtain the derivatives of order $n$ in the $\nu$ initial conditions.

While this method is practically straightforward and very robust, several comments and cautions are in order. First, if the step sizes in the original integration scheme are chosen to be sufficient to obtain the final conditions with sufficient
accuracy, this does not necessarily guarantee any accuracy of the derivatives obtained by this approach. In fact, in most practical cases we observe that the accuracy of the derivatives decreases rapidly with order. One straightforward and robust way to circumvent this problem in practice is to utilize an integration scheme with automatic step size control, where the norm utilized in the accuracy control is replaced by the corresponding norm in Eq. (2.68). In this way, the automatic step size control assures that all derivatives in the components of the DA vector are determined with suitable accuracy. While this leads to a straightforward algorithm, it often entails significantly smaller step sizes than in the original algorithm, but is unavoidable in order to obtain accurate derivatives.

Another practical difficulty arises when parts of the functional dependencies in the integration scheme are not differentiable. This situation, that often arises when direct use of measured field data is made, can sometimes lead to very inaccurate or even wrong values for higher derivatives, unless suitable precautions are taken, as in the representation of the field by the smooth model in Eq. (3.20).

Altogether, the method is robust and straightforward to implement, but has potential pitfalls. Furthermore, its computational expense is proportional to the expense of the original integrator times the computational expense for the elementary DA operations, and for high orders and many variables can become significant. It has been implemented in the code COSY INFINITY (Berz 1997a; et al.) as well as a number of other recent codes (Yan 1993; Yan and Yan 1990; van Zeijts and Neri 1993; Michelotti 1990; Davis, Douglas, Pusch, and Lee-Whiting 1993).

5.4.2 DA Solvers for Differential Equations

Besides differentiation through the numerical integrator, the various DA-based ODE solvers discussed in Section 2.3.4 often represent significant advantages. The algorithm based on fixed-point iteration (Eq. 2.115), a natural approach within the DA framework, can outperform the integrator discussed in the previous section in speed, especially for ODEs for which the right-hand sides consist of a large number of arithmetic operations. Similar to the previously discussed integrators, it offers straightforward step size control via the use of the DA norm (Eq. 2.68).

For autonomous systems, which occur, for example, in the main field of particle optical elements, the use of the propagator (Eq. 2.120)

\[
\mathcal{Z}_f = \sum_{i=1}^{\infty} \frac{t^i \cdot L^i}{i!} \mathcal{I}
\]

is particularly suitable. In this case, the right-hand side \( \mathcal{Z}_f \) has to be evaluated only once per step, and each new order in the power series requires only the application of the derivation operation and is hence only a small multiple of the
cost of evaluation of $\tilde{f}$. Therefore, this method is most efficient at high orders and large time steps. In the COSY INFINITY code, step sizes are fixed and orders adjusted dynamically, typically falling in a range between 25 and 30. Altogether, the DA-based ODE solvers are the main integration tools in the COSY INFINITY code (Berz 1997a; et al.) and represent the method of choice where applicable.

5.4.3 Fast Perturbative Approximations

In the following, we develop fast approximate methods for the computation of maps for which the use of the autonomous solver is not applicable, and which would otherwise require more time-consuming approaches. The tools are perturbative in that they are applicable for various systems near a reference system to be specified. In particular, the method allows efficient treatment of fringe field effects.

Because of the simplifications available for autonomous systems, the effect of a particle optical device is represented traditionally by a field-free drift and a main-field region. If effects of the $s$ dependent parts of an element, so called fringe-field effects, are considered, they are represented by a fringe-field map, which is sandwiched between the drift and the main-field map at the position $s_0$. Hence, the fringe-field map consists of a negative drift to the region where the field vanishes, the map through the varying field, and the application of an inverse main-field map back to $s_0$ as shown in Fig. 5.8. So the fringe-field map represents the necessary corrections to the simple step function field model described by

$$B_{mf}(x, y, s) = \begin{cases} \tilde{B}(x, y, s_m) & \text{for } s \text{ in the main field} \\ 0 & \text{for } s \text{ outside the main field} \end{cases}$$

where $s_m$ describes the center of the main field. The abrupt change of the field in this model of course violates Laplace’s equation and cannot therefore represent a physical system. To describe a realistic system, the main-field map must be
composed with fringe-field maps, which describe the connection of the main-field to the field-free region outside the element. As outlined in the previous section, the main-field map of optical elements can be computed more easily than that of the fringe fields; the situation is similar in older low-order codes utilizing analytically derived formulas (Matsuo and Matsuda 1976; Wollnik 1965; Brown 1979a; Dragt, Healy, Neri, and Ryne 1985; Berz, Hofmann, and Wollnik 1987).

As mentioned previously, the fringe-field map $M_{ff}$ is defined as a correction to be inserted at the edge of the element, which can be formalized as follows. Let $s_0$ denote the effective field boundary at the entrance of the element, $s_-$ a position so far before the optical device that the field can be neglected, and $s_+$ a position so far inside the element that $B(x, y, s)$ changes very little with $s$. Let the map $M_{mfs_0 \rightarrow s_+}$ describe particle motion through the main field given in Eq. (5.76) from the effective field boundary to $s_+$. The fringe-field map is constructed in such a way that a drift $\vec{D}_{s_- \rightarrow s_0}$ from $s_-$ to the effective field boundary composed first with $M_{ff}$ and then with $M_{mfs_0 \rightarrow s_+}$ yields the transfer map $M_{s_- \rightarrow s_+}$ from $s_- \rightarrow s_+$:

$$M_{s_- \rightarrow s_+} = M_{mfs_0 \rightarrow s_+} \circ M_{ff} \circ \vec{D}_{s_- \rightarrow s_0}.$$  \hspace{1cm} (5.77)

Hence the fringe-field map has the form

$$M_{ff} = M_{mfs_0 \rightarrow s_+}^{-1} \circ \vec{D}_{s_- \rightarrow s_0}^{-1}.$$  \hspace{1cm} (5.78)

Computing fringe-field maps requires the computation of the map $M_{s_- \rightarrow s_+}$ of a system where $\vec{B}(x, y, s)$ and, hence, the differential equation depends on $s$. While the resulting computational effort is substantially greater, ignoring the fringe-field effects unfortunately leads to substantial errors in the nonlinearities of the element.

The importance of fringe fields becomes apparent when realizing that many nonlinear properties of an electric or magnetic field are due to the dependence of the field on $s$, as seen in Eq. (3.9). Many nonlinear contributions arise only because of the non-vanishing $s$ derivatives. However, the functions involved and also their derivatives can be quite complicated; one frequently used model is the so-called Enge function, which has the form

$$E(s) = \frac{1}{1 + \exp(b_{k,0} + b_{k,1}(s/a) + b_{k,2}(s/a)^2 + \ldots)},$$  \hspace{1cm} (5.79)

in which $a$ is the aperture of the device under consideration, and $b_{k,i}$ are real coefficients modeling the details of the field’s fall-off.

A careful treatment of fringe-field effects is imperative for a detailed study of nonlinear effects, and the advantages of very fast DA evaluation of propagators can be used most dramatically with efficient fringe-field approximations.

Any approximation for such fringe-field effects should satisfy various requirements. It should:
1. lead to order \(n\) symplectic maps
2. represent the \(s\) dependent element well for a wide range of apertures
3. be usable for arbitrary orders.

The simplest approximation, already described, is SCOFF, where \(s\) dependent fields are simply ignored. As illustrated previously, this method strongly violates the accuracy requirement and point 2. The impulse approximation (Helm 1963) used in the code TRANSPORT (Brown 1979a) violates points 2 and 3, and the method of fringe-field integrals (Hartmann, Berz, and Wollnik 1990; Wollnik 1965) used in the computer code GIOS (Wollnik, Hartmann, and Berz 1988) violates points 1 and 3.

The general problem is to determine the transfer map of interest for a beam with reference particle of energy \(E\), mass \(m\), and charge \(q\) in a magnetic or electric particle optical device. The device is characterized by a size parameter \(A\), a reference field strength \(F\), and, possibly, additional parameters \(\delta\). Thus, the task is to find the transfer map

\[
\mathcal{M}^{E,m,q,A,F}(z,\delta),
\]  

(5.80)

that will be achieved by relating it through a sequence of transformations to a suitably chosen previously computed and stored reference map. The SYSCA method (Hoffstätter 1994; Hoffstätter and Berz 1996b) outlined in the following relies on two different scaling mechanisms, one based on geometric observations, and the other relying on the linear relation between rigidity of a particle and the field.

The first scaling method used in the determination of the map of a general element is based on a simple geometric observation. Assume a certain space-dependent field and an orbit through it are given. If the geometry of the field is scaled up by a factor \(\alpha\) and, simultaneously, the field strength is scaled down by the factor \(\alpha\), then the original orbit can be scaled up by the factor \(\alpha\) along with the geometry of the device. The reason for this phenomenon is that the momentary radius of curvature of the orbit, which is geometric in nature, is inversely proportional to the field, which follows directly from the Lorentz equation. If a trajectory described by \(x(t)\) and \(p(t)\) satisfies

\[
\frac{dp}{dt} = q \left( \frac{dx}{dt} \times \vec{B}(x) + \vec{E}(x) \right),
\]  

(5.81)

then a scaled trajectory \(\vec{X}(t) = \alpha \vec{x}(t/\alpha)\) and \(\vec{P} = \vec{p}(t/\alpha)\) satisfies

\[
\frac{d\vec{P}}{dt} = q \left( \frac{d\vec{X}}{dt} \times \frac{1}{\alpha} \vec{B}(\vec{X}/\alpha) + \frac{1}{\alpha} E(\vec{X}/\alpha) \right).
\]  

(5.82)

A limitation to this approach is that the shape of the field is not only determined by the geometry generating it, but also by possible saturation effects that depend
If the size of an element is scaled by a factor $\alpha$ and simultaneously the strength of the field is scaled by a factor $1/\alpha$, then coordinates of particle trajectories scale with the factor $\alpha$.

on the strength of the field. This limits the allowed factor $\alpha$ to a size where changes of saturation can be ignored.

It is also important to note that once the ratio of length to aperture of a device exceeds a certain minimum, the exact shape of the fringe field is almost unaffected by the actual length of the device. Therefore, for the treatment of fringe fields, in good approximation the aperture of the element can be used as size parameter $A$.

For the actual use of the method, it is important to observe that only geometric quantities associated with the particle, like positions, slopes, and lengths of trajectories, scale with the geometry, while the canonical momenta do not scale properly. Thus before scaling it is necessary to transform the map to purely geometric coordinates like those used in the TRANSPORT code (Brown 1979a). The transformation between these two sets of coordinates depends on the energy $E_0$ and the mass $m_0$ of the reference particle, and is denoted by $\mathbf{T}(E_0, m_0)$. The coordinates are denoted by $\mathbf{z}_{E_0} = (x, y, b, \delta_E, \tau)$ and $\mathbf{z}_{p_0} = (x', y', l, \delta_p)$ and the transformation is given by

\begin{align*}
x' &= \frac{a}{\sqrt{(\frac{a}{p_0})^2 - a^2 - b^2}}, \\
y' &= \frac{b}{\sqrt{(\frac{a}{p_0})^2 - a^2 - b^2}}, \\
l &= l_t - \frac{v}{v_0} \left[ \frac{2 + \eta_0}{1 + \eta_0} \left( \tau - \tau_t \right) + \left( \frac{v}{v_0} - 1 \right) s \right], \\
\delta_p &= \sqrt{\frac{(E_0(1 + \delta_E))^2 + 2E_0mc^2(1 + \delta_E)}{p_0c} - 1}, \tag{5.83}
\end{align*}

which has the inverse

\begin{align*}
a &= \left( \frac{p}{p_0} \right) \frac{x'}{\sqrt{1 + x'^2 + y'^2}}, \\
b &= \left( \frac{p}{p_0} \right) \frac{y'}{\sqrt{1 + x'^2 + y'^2}},
\end{align*}
\[ \tau = \tau_i - \frac{v_0}{v} \left( 1 + \frac{1}{\eta_0} \left( l - l_i - \frac{v}{v_0} - 1 \right) s \right), \]
\[ \delta_E = \frac{\sqrt{(p_0c(1 + \delta_p))^2 + (mc^2)^2} - mc^2}{E_0} - 1. \] (5.84)

The change of coordinates can be performed conveniently to arbitrary order in DA following Eq. (4.5). It is worthwhile to point out that in order to perform the transformation, the knowledge of the total arc length \( s \) of the system under consideration as well as the mass and energy of the reference particle is required; thus, these quantities have to be stored along with the reference map. In geometric coordinates, the map \( S_\alpha \) performing the scaling is characterized by

\[ x_2 = x_1 \alpha, \quad y_2 = y_1 \alpha, \quad l_2 = l_1 \alpha, \quad \delta_{p2} = \delta_{p1}; \] (5.85)

if there are any parameters \( \delta \), their scaling behavior must also be considered.

The geometric scaling thus allows expression of a map that is associated with the size scale \( A \), in terms of a stored reference map whose size scale is \( A^* = \alpha \cdot A \). This is accomplished by the transformations

\[ \tilde{M}^{E,m,0,F,A}(\vec{z}_E, \vec{\delta}) = \tilde{T}^{-1} \circ \tilde{S}^{-1} \circ \tilde{T} \circ \tilde{M}^{E,m,A^*,F/\alpha}(\vec{z}_E, \vec{\delta}) \circ \tilde{T}^{-1} \circ \tilde{S}_\alpha \circ \tilde{T}. \] (5.86)

Since the stored reference map has to be evaluated at \( F/\alpha \), it is clear that the reference map has to be known as a function of the field strength.

The next step is to transform the properties of the reference particle to those stored in the reference file. To this end, the rigidity \( \chi \) of the reference particle of interest is computed and compared to that of the stored map \( \chi^* \); since electric and magnetic rigidities depend on the quantities \( E, q, m \) in different ways, this requires that electric and magnetic fields not be present simultaneously. In the following, we discuss the case of the magnetic field in detail and only briefly mention the electric case. Let \( \beta = \chi^*/\chi \) be the ratio of the rigidity associated with the stored map and the map under consideration. Because of \( vB = qE \times B \), a simultaneous scaling of magnetic rigidity and magnetic field has no influence on the orbit, we have \( \tilde{M}^{E,m,0,A^*,F/\alpha}(\vec{z}_E, \vec{\delta}) = \tilde{M}^{E^*,m^*,A^*,F/\alpha}(\vec{z}_E, \vec{\delta}) \). The change of a trajectory induced by a relative energy deviation \( \delta_E \) depends on the energy \( E \) of the reference particle. This cannot be true, however, for \( \delta_p \). Due to the scaling law for magnetic rigidity, a relative momentum deviation \( \delta_p \) creates the same changes in a trajectory, no matter which reference momentum \( p \) is used. Thus, the full transformation to the reference map is obtained as

\[ \tilde{M}^{E, m, 0, F}(\vec{z}_E, \vec{\delta}) = \tilde{T}^{-1}(E, m) \circ \tilde{S}^{-1} \circ \] (5.87)
\[ \{ \tilde{T}(E^*, m^*) \circ \tilde{M}^{E^*, m^*, A^*, F}(\vec{z}_E, \vec{\delta}, \vec{F}) \circ \tilde{T}^{-1}(E^*, m^*) \} \circ \tilde{S}_{\beta/\alpha} \circ \tilde{S}_\alpha \circ \tilde{T}(E, m). \]
Besides the dependence of the original map on the parameters \( \delta \), its dependence on the field \( F \) has to be known. While the exact dependence of the map on the field is usually difficult to obtain, the DA method conveniently allows determination of the expansion in terms of the field strength.

For an electric field of strength \( F \) the trajectory does not change if the quantity \( F q / \nu_p \) does not change, due to \( v F \delta = q \vec{E} \). Therefore, TRANSPORT coordinates \( \vec{z}_p \) with \( \delta_p \) are not appropriate but \( \delta_{vp} \) must be used, which denotes the relative deviation of \( \nu p \) from the corresponding value for the reference particle.

Even though this expansion can be obtained to rather high order, it still represents a source of errors, and hence a study of the influence of these errors is warranted. The first question is that of the accuracy of the expansion; for this purpose we analyze the range of values the quantity

\[
\vec{F} = F \cdot \frac{\beta}{\alpha}
\]  

(5.88)
can assume; this establishes how far away from a chosen expansion point the extrapolation will have to be made. However, as it turns out, the quantity \( \vec{F} \) has a rather simple geometric meaning. Note that both in the process of size scaling and in the process of rigidity scaling, the total deflection of a particle transversing the field at the aperture is not changed. Thus, the quantity \( \vec{F} \) plays the role of a universal strength parameter.

The other important consideration in the process of approximating the field dependence in terms of an expansion is the question of symplecticity. Even if the errors produced by inserting into the truncated polynomial are minor, without additional considerations they violate the symplectic symmetry of the map.

This problem can be avoided by storing a symplectic representation of the map. For the nonlinear part of the map, it appears advantageous to choose a one-operator flow representation (Eq. 4.79) using the pseudo–Hamiltonian, which can be determined from the map

\[
\vec{M}(\vec{z}_E, \vec{F}) = L(\vec{F})e^{P(\vec{z}_e, \vec{F})}.
\]  

(5.89)

On the other hand, for the linear part this representation just contains the linear matrix in ordinary nonsymplectic form. To preserve the symplecticity of the linear part, it is advantageous to represent it in terms of a generating function (Eq. 4.81), which again can be conveniently calculated from the map.

There are a variety of ways to extend the method of symplectic scaling. First, note that the required knowledge of the dependence of the map on a relative field change \( \delta_F \) can be indirectly obtained from the conventional map itself. To this end, we can express the chromatic dependence of the map, not in terms of the conventional energy deviation \( \delta_E \), but in terms of the momentum deviation \( \delta_p \), and substitute

\[
\vec{M}^{E:m,q:A:F}(\vec{z}_E, \delta_F) = \vec{T}(E, m) \circ \vec{M}^{E:m,q:A:F}(z, z', y, y', l, \delta_p/(1 + \delta_F))
\]  

(5.90)
This observation is particularly useful for the practical use of the method since it does not require any special setup to determine the stored map.

Similarly, the two scaling properties can be used to compute the map’s dependence on a relative change of aperture \( \delta_A \), mass \( \delta_m \), and charge \( \delta_q \). Therefore, no special parameters \( \vec{\delta} \) have to be introduced to compute these dependencies if they are desired, and we write the most general parameter dependent map as 

\[ \vec{M}_{E,m,q,A,F}(\vec{z}_E, \delta, \delta_m, \delta_q, \delta_A, \delta_F). \]

Another possible extension is the use of the parameters \( \vec{\delta} \) for the description of other degrees of freedom of the field under consideration. These could include details about the fall off, or about the geometric form of the effective field boundary.

The last topic is of great practical importance and can also be treated conveniently by rotating the fringe-field map of a wedge dipole appropriately, as discussed in the following.

Finally, for practical considerations it is sufficient to store only maps of entrance fringe fields. Given the entrance fringe field map \( \vec{L}_o(\exp(P;P;\vec{z})) \), the exit fringe-field map is described by the reversed map in (Eq. 4.8). In addition, if a representation approximates maps of \( 2 \nu \) poles with fields close to \( B \), then a rotation by an angle of \( 180/\nu^2 \) allows approximations close to the field \( -B \).

To avoid the computation of a reference file for different possible edge angles and curvatures, a further approximation is used. The effect of the edge shape is approximated by first applying the fringe-field map of a straight edge dipole, and then taking curvatures up to second order into account analytically. Higher-order curvatures are evaluated with nonlinear kicks.

The following table demonstrates the applicability of this approximation. We used a dipole of radius 2 m, a bend angle of 30\(^\circ\), and an aperture of one inch. The Taylor coefficients \((a,xa)\) and \((x,xaa)\) were computed with SYSCA (left) and

<table>
<thead>
<tr>
<th>angle</th>
<th>((a,xa)) m</th>
<th>((x,xaa))</th>
</tr>
</thead>
<tbody>
<tr>
<td>5(^\circ)</td>
<td>-0.1360314E-02</td>
<td>-0.1368305E-02</td>
</tr>
<tr>
<td>10(^\circ)</td>
<td>-0.7231982E-03</td>
<td>-0.7253955E-03</td>
</tr>
<tr>
<td>15(^\circ)</td>
<td>-0.1033785E-06</td>
<td>-0.2891228E-08</td>
</tr>
<tr>
<td>20(^\circ)</td>
<td>-0.1718367E-02</td>
<td>-0.1721275E-02</td>
</tr>
<tr>
<td>25(^\circ)</td>
<td>-0.9628906E-02</td>
<td>-0.9643736E-02</td>
</tr>
<tr>
<td>30(^\circ)</td>
<td>-0.2977263E-01</td>
<td>-0.2981580E-01</td>
</tr>
<tr>
<td>5(^\circ)</td>
<td>-0.6524050E-01</td>
<td>-0.6520405E-01</td>
</tr>
<tr>
<td>10(^\circ)</td>
<td>0.5269389E-03</td>
<td>0.5795750E-03</td>
</tr>
<tr>
<td>15(^\circ)</td>
<td>0.7179696E-01</td>
<td>0.7179678E-01</td>
</tr>
<tr>
<td>20(^\circ)</td>
<td>0.1463239</td>
<td>0.1461203</td>
</tr>
<tr>
<td>25(^\circ)</td>
<td>0.2187553</td>
<td>0.2180152</td>
</tr>
<tr>
<td>30(^\circ)</td>
<td>0.2775432</td>
<td>0.2755090</td>
</tr>
</tbody>
</table>
with accurate numerical integration in DA (right) for different edge angles. In all examples the entrance and the exit edge angle are equal.

To approximate the effects of superimposed multipoles, we compute fringe-field maps of the separate multipoles via SYSCA. These fringe-field maps are then composed to a single map, to approximate the fringe-field map of the instrument with superimposed multipoles. While this approximation may appear crude, it is often quite accurate, as shown in the following table. SYSCA (left) and DA integration (right) was used to compute coefficients of the fringe-field map of a magnetic quadrupole that is superimposed with a magnetic hexapole. The instrument has an aperture of one inch and was 0.5 m long. The pole-tip field of the quadrupole was $1T$ and the pole-tip field $B_H$ of the hexapole is given in the table.

<table>
<thead>
<tr>
<th>$B_H/T$</th>
<th>$(a, xa)m$</th>
<th>$(x, aaa)/m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>0.1</td>
<td>-2.54411</td>
<td>-2.54412</td>
</tr>
<tr>
<td>0.2</td>
<td>-5.08823</td>
<td>-5.08824</td>
</tr>
<tr>
<td>0.3</td>
<td>-7.63235</td>
<td>-7.63236</td>
</tr>
<tr>
<td>0.4</td>
<td>-10.17647</td>
<td>-10.17649</td>
</tr>
<tr>
<td>0.5</td>
<td>-12.72058</td>
<td>-12.72061</td>
</tr>
</tbody>
</table>

For a variety of examples showing the validity and accuracy of the SYSCA approach for various specific systems, refer to (Hoffstätter 1994; Hoffstätter and Berz 1996b).