SINGLE PARTICLE LINEAR AND NONLINEAR DYNAMICS

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Abstract

I will give a comprehensive review of existing particle tracking tools to assess long-term particle stability for small and large accelerators in the presence of realistic magnetic imperfections and machine misalignments. The emphasis will be on the tracking and analysis tools based upon the differential algebra, Lie operator, and “polymorphism”. Using these tools, a uniform linear and non-linear analysis will be outlined as an application of the normal form.

INTRODUCTION

Computational tools play an important role in the design and operation of modern accelerators which are pushed to the very limits of their performance. During the design stage, the computer programs are routinely used to match the beam optics, compensate for the chromatic effects, analyze the machine tolerance, and estimate the stability of a single particle. In commissioning and operation, the codes are used to build realistic accelerator models, control the closed orbit, and correct linear optics.

Since the physics of single-particle dynamics starts from the Lorentz force and the relativistic equations of motion, all computer programs that describe the motion of charged particles in accelerators have the same description given the electric and magnetic field. They can differ only when physical approximations are made for magnetic elements in the machine. Hence, we can classify these computer programs according to what kind of presentations are chosen for the magnetic elements. Generally speaking, there are three such presentations: Taylor map [1], Lie factors [2], and symplectic integrators [3]. Indeed they provide almost all engines in commonly used accelerator codes; for example, Lie factors in MARYLIE [4], Taylor map in MAD [5], and Ruth integrator [6] in LEGO [7].

It is well known that these presentations can be transformed from one to another. For instance, the differential algebra [8] provides us an efficient and accurate method to extract a truncated Taylor expansion from symplectic integrators. Then the Taylor map can be transformed into the exponential factors using the Dragt-Finn procedure [9].

In their abstract forms, all three presentations are perfect for tracking a charged particle through a lattice of magnetic elements. In practice however, both Taylor map and Lie operator have to be truncated to a certain order in terms of the canonical variables during the evaluation of the map. The truncation causes the violation of the symplecticity, which is the fundamental underlining symmetry of the Hamiltonian system. This violation of symmetry could lead to artificial growth or damping of the amplitude of the particle trajectory. As a result, the codes based on the truncated transfer maps can not be reliably used to estimate the stability of a particle in circular accelerators.

On the other hand, the explicit canonical integrator allows us to exactly evaluate an approximated Hamiltonian at each integration step. These solvable solutions preserve the symplecticity of the system. Since the numbers of the solvable solutions are very limited, the engines of the codes are relatively easy to describe and understand. In short, symplecticity and simplicity are the main reasons why the codes based on the explicit canonical integrators have become popular recently. Modern codes using these integrators are the main subject in this paper.

In the first section, we will introduce a Hamiltonian for a single particle in static magnetic field and the general Lie transformation that is associated with the Hamiltonian system. Then we will discuss solvable solutions and symplectic integrators. Finally we will outline a general and uniform approach to both linear and nonlinear analysis of lattices with periodic magnetic elements.

HAMILTONIAN

In a planar curved coordinate system characterized by radius of curvature $\rho$, the Hamiltonian, using the distance $s$ along the curve as the independent variable for a charged particle moving in a static magnetic field, is given by: [10]

\[
H(x, p_x, y, p_y, \delta, l; s) = -a_s - \frac{x}{\rho} \sqrt{(1 + \delta)^2 - (p_x - a_x)^2 - (p_y - a_y)^2},
\]

Figure 1: The planar curved coordinate system.
where \( a_{x,y,s} = eA_{x,y,s}/cp_0 \) are scaled components of the vector potential along axes \( x,y,s \), respectively; \( p_x, p_s \) are the transverse canonical momenta scaled by a reference momentum \( p_0 \), \( \delta = (p - p_0)/p_0 \), and \( l = vt \) is the path length. Note that the Hamiltonian in Cartesian coordinates can be obtained simply by taking the limit as \( \rho \to \infty \) in Eq. (1).

Formally, the solution of the Hamiltonian’s equations from the initial canonical coordinates \( z(s_1) \) to the final ones \( z(s_2) \) can be expressed as

\[
z(s_2) = \mathbb{S}e^{-\int_{s_1}^{s_2} H(z,s) \, ds} z(s_1) = \prod_{s_1 < s < s_2} (e^{-\int_{s}^{s+\delta} (e^{-H(z,s) \, ds})} z(s_1). \tag{2}
\]

Here the infinitesimal Lie transformation: \( e^{-\int_{s}^{s+\delta} (e^{-H(z,s) \, ds})} \) is defined using the Poisson brackets [2] and the symbol \( \mathbb{S} \) denotes the \( s \)-ordered product similar to the time-ordered product in quantum field theory, but with an opposite ordering to keep the convention consistent with mapping, namely, smaller \( s \) on the left.

If the Hamiltonian does not explicitly depend on \( s \), the product of infinitesimal transformations can be combined into a single Lie transformation,

\[
z(s_2) = e^{-\int_{s_1}^{s_2} H(z,s) \, ds} z(s_1), \tag{3}
\]

where \( L = s_2 - s_1 \). It can be applied to the body of a magnet where the field is constant with respect to \( s \).

**A SECTOR BEND**

Since the bending magnets, which guide the charged particles circulating in the ring, are the most common elements in accelerators, let’s take a horizontal dipole magnet with uniform field \( B_0 \) as our starting point. By properly choosing a gauge [11], we have \( A_x = A_y = 0 \) and \( A_z = -B_0 x - B_0 x^2/2 \rho \). Substituting the vector potential into Eq. (1), we obtain the Hamiltonian of a sector bend,

\[
H_b(z) = b_0 x + b_0 x^2/2 \rho - (1 + x/\rho) \sqrt{(1 + \delta)^2 - p_x^2 - p_y^2}, \tag{4}
\]

where \( b_0 = eB_0/p_0c \). Though the Hamiltonian seems complicated, its equations are solved exactly [12]. Noting \( p_s(p_x, p_y) = \sqrt{(1 + \delta)^2 - p_x^2 - p_y^2} \), the solution is

\[
\begin{align*}
x^f &= \frac{1}{b_0} p_s(p_x', p_y') - \frac{\rho}{b_0} \frac{dp_f}{ds} - \rho \\
p_x^f &= p_x \cos(\phi) + [p_s(p_x, p_y) - b_0(\rho + x)] \sin(\phi)/\rho \\
y^f &= y + \frac{p_y}{b_0}(\rho + \phi) \\
p_y^f &= p_y \\
\delta^f &= \delta \\
l^f &= l + (1 + \delta) \frac{\delta}{\rho} \phi.
\end{align*}
\]

where

\[
\phi = \arcsin\left(\frac{p_x}{p_s(0, p_y)}\right) - \arcsin\left(\frac{p_y'}{p_s(0, p_y)}\right).
\]

Since we did not use the so-called paraxial approximation, which assumes that \( p_x \) and \( p_y \) are much smaller than 1 and expand the square root in the Hamiltonian, this solution is applicable even to extremely small rings.

![Schematic of a sector bend](image.png)

**Figure 2: Two periodic orbits \((x^0, p_0^0) = (0, 0.2, p_y = \delta = 0, \text{and } 1/b_0 = \rho = 1 \text{m})\) as solutions of Eq. (4) in the global coordinate system.**

Although the solution is complicated in the local curved coordinate system, it describes the well-known spiral motion of a charged particle in a constant magnetic field. As plotted using Eqs. (5) in Fig 2, two particles execute cyclotron motion periodically. This system is integrable and the nonlinear kinematic terms in Eq. (4) themselves do not lead to any nonlinear resonances to the system.

**SYMPLECTIC INTEGRATORS**

One of most important achievements in the history of modern accelerator physics was the discovery of the alternating-gradient principle [11]. That principle leads us to introduce quadrupole magnets into circular accelerators. To describe the magnetic field inside a quadrupole magnet or other type of magnets we use the harmonic expansion,

\[
B_y + iB_x = \sum_{n=1}^{\infty} (b_n + ia_n)(x + iy)^{n-1}, \tag{6}
\]

where \( b_n, a_n \) are the normal and skew components respectively. Eq. (7) also describes the magnetic errors inside the body of magnets. For instance, \( b_2 \) is the quadrupole component and \( b_3 \) presents a normal sextupole component which usually is the largest error in a dipole magnet. The corresponding vector potential is \( A_x = A_y = 0 \) and

\[
A_n^1(x,y) = -Re\left(\sum_{n=1}^{\infty} (b_n + ia_n)(x + iy)^n\right). \tag{7}
\]

Using this vector potential, along with the one for the perfect sector bend in the previous section, we have the
Hamiltionian for realistic bending magnets including the multipole components
\[ H(z) = H_b(z) + H_m(x, y), \quad (8) \]
where \( H_m(x, y) = -eA_m^s(x, y)/p_0c. \) In general, this Hamiltonian system is not solvable and some kind of approximation has to be made to solve Hamiltonian’s equations.

Note that \( H_m(x, y) \) itself can be solved because it depends only on the coordinates not on the canonical momenta. The momenta change due to \( H_m(x, y) \) is commonly called a kick. Based on the separately solvable Hamiltonian systems \( H_b(z) \) and \( H_m(x, y) \), one can construct a second-order symplectic integrator by lumping the integrated kick at the middle of the magnet. Expressing the approximation in terms of Lie transformations, we have
\[ e^{-\mathcal{H}:\mathbf{L}} = e^{-\mathcal{H}_b:\mathbf{L}} e^{-\mathcal{H}_m:2\mathbf{L}} e^{-\mathcal{H}_b:2\mathbf{L}} + O(L^3), \quad (9) \]
where \( L = \theta \rho \) is the arc length of the sector magnet and \( \theta \) is the bending angle. The error due to this approximation is on the order of \( L^3 \), which is easily estimated using the Baker-Cambell-Hausdorf formula \[ e^{f} e^{g} = e^{f + g + [f; g] + \ldots}, \quad (10) \]
here the bracket \([,] \) denotes the Poisson bracket.

To reduce the error further, one can first divide the magnet into many identical segments and then use the integrator for each segment. It is worth noting that, in the limit of an infinite number of segments, the residual error reduces to an zero and the approximated solution becomes the exact one.

In general, it is an approximate solution but preserves the simplicity during the integration because the solutions of both \( H_b \)'s and \( H_m \)'s are symplectic.

However, the way to build second-order integrators from the Hamiltonian in Eq. (8) is far from unique. In fact, we can split it into three solvable ones as following
\[ H(z) = H_d + H_y + H_k, \quad (11) \]
where
\[ H_d = -\sqrt{(1 + \delta)^2 - p_x^2} - p_y^2, \]
\[ H_y = -\frac{x}{\rho} \sqrt{(1 + \delta)^2 - p_x^2} - p_y^2, \]
\[ H_k = b_0 x + b_0 \frac{p_x^2}{2 \rho} - eA_m^s(x, y)/p_0c. \quad (12) \]
It is obvious that \( H_d \) and \( H_k \) are solvable since they either depend on the coordinate or its conjugate momentum but not on both. The solution of the \( H_y \)'s is not so trivial. One can start to solve \( p_x \) and \( p_y \) as \( \sqrt{(1 + \delta)^2 - p_x^2} - p_y^2 \) and then use the fact that \( xp_y \) is a constant of the motion. The solution is
\[ x^f = \frac{xp_y}{\cos(\frac{\theta}{\rho})[p_y - p_x \tan(\frac{\theta}{\rho})]}, \]
\[ y^f = \frac{xp_y \tan(\frac{\theta}{\rho})}{[p_y - p_x \tan(\frac{\theta}{\rho})]}, \]
\[ p_x^f = p_x \cos(\frac{\theta}{\rho}) + p_y \sin(\frac{\theta}{\rho}), \]
\[ y^f = \frac{xp_y \tan(\frac{\theta}{\rho})}{[p_y - p_x \tan(\frac{\theta}{\rho})]}, \]
\[ p_y^f = p_y, \]
\[ \delta^f = \delta. \]
\[ l^f = l + \frac{x(1 + \delta) \tan(\frac{\theta}{\rho})}{[p_y - p_x \tan(\frac{\theta}{\rho})]}. \quad (13) \]
This solution can be interpreted [13] as a rotational Lie transformation around the y axis with an angle \( -s/\rho \).

Based on these solvable solutions, we obtain another second-order integrator
\[ e^{-\mathcal{H}:L} = e^{-\mathcal{H}_d:2\mathbf{L}} e^{-\mathcal{H}_y:2\mathbf{L}} e^{-\mathcal{H}_k:2\mathbf{L}} + O(L^3). \quad (14) \]
Here, once again, we derive the main algorithms discovered first in TEAPOT [14]. \( e^{-\mathcal{H}_d:2\mathbf{L}} \) provides a rotation around the \(-y\) axis with half of the bending angle before and after the kick. Of course, our approach is based on the local Hamiltonian instead of the global geometry. It is trivial to extend this to the case of vertical bends.

In addition to the second-order integrators, we can construct even higher order integrators [15] based on symmetrically arranged second-order integrators. In particular, given a second-order integrator \( S_2(L) \), such as the one described by Eq. (9) or (14), one can construct the fourth-order integrator (Ruth integrator)
\[ S_4(L) = S_2(x_1 L) S_2(x_0 L) S_2(x_1 L), \quad (15) \]
where \( x_0 = -2\pi/(2 - 2\xi), x_1 = 1/(2 - 2\xi). \) To make more efficient integration, we can replace the fourth-order integrator with the second-order one with a smaller number of segments. In a typical circular accelerator, we find that several segments of the second-order integrators are adequate for dipole magnets however for quadrupole magnets, one needs a few segments of the fourth-order ones.

**LINEAR ANALYSIS**

It is well known that the one-turn map at any given location \( s \) in a circular accelerator can be described using the Courant-Synder parameters: \( \beta(s), \alpha(s), \) and \( \gamma(s) \) [11],
\[ M = \begin{pmatrix}
\cos \mu + \alpha \sin \mu & \beta \sin \mu \\
-\gamma \sin \mu & \cos \mu - \alpha \sin \mu
\end{pmatrix}, \quad (16) \]
where \( \mu = 2\pi \nu \) is the entire phase advance in the ring and \( \nu \) is the betatron tune. The matrix \( M \) can be transformed into a simple rotation with a canonical transformation,
\[ M = A \cdot R \cdot A^{-1}, \quad (17) \]
where $A^{-1}$ is a canonical transformation that normalizes the phase coordinates:

$$A^{-1} = \begin{pmatrix} \frac{1}{\sqrt{\beta}} & 0 \\ \frac{1}{\sqrt{\beta}} & 0 \end{pmatrix} , \quad A = \begin{pmatrix} \sqrt{\beta} & 0 \\ \sqrt{\beta} & 1 \end{pmatrix} ,$$

(18)

and $R(\mu)$ is a two-dimensional rotation matrix

$$R(\mu) = \begin{pmatrix} \cos \mu & -\sin \mu \\ \sin \mu & \cos \mu \end{pmatrix} .$$

(19)

It is worth noting that the transformation $A$ is unique only up to a global phase $\psi$ since the matrix

$$\tilde{A} = A \cdot R(\psi),$$

(20)

could also normalize the phase coordinates. However, one can easily show that the Courant-Snyder parameters are actually independent of the arbitrary phase $\psi$. They can be computed using the elements of matrix $\tilde{A}$

$$\beta = \tilde{A}_{11} + \tilde{A}_{22},$$

$$\alpha = -(\tilde{A}_{11}\tilde{A}_{21} + \tilde{A}_{12}\tilde{A}_{22}),$$

$$\gamma = \tilde{A}_{21}^2 + \tilde{A}_{22}^2.$$  

(21)

Although $\psi$ is arbitrary and meaningless at any given location $s$, the phase different $\delta \psi_{12} = \psi(s_2) - \psi(s_1)$ can be identified as the betatron phase advance between two points $s_1$ and $s_2$ if we relate the two transformations as follow:

$$\tilde{A}(s_2) = A(s_2) \cdot R(\delta \psi_{12}) = M_{12} \cdot A(s_1),$$

(22)

where $M_{12}$ is the linear transfer matrix between $s_1$ and $s_2$. In fact, one can easily show that $A(s_2)$ and $\tilde{A}(s_2)$ constructed from Eq. (22) both normalize the phase coordinates at position $s_2$ using the fact that the betatron tune $\nu$ is a global invariant in the ring. The Courant-Snyder parameters can be calculated using Eq. (21). In addition, the phase advance is given by

$$\delta \psi_{12} = \arctan(\tilde{A}_{12}/\tilde{A}_{11}).$$

(23)

Figure 3: Illustration of the relationship between the physical and normalized rings.

The process of normalizing coordinates is shown in Fig. 3. In the normalized ring, phase vector $(x, p_x)$ rotates according to the phase advance. Eq. (22) provides us a simple way to propagate the lattice functions $\alpha, \beta, \gamma,$ and $\psi$ throughout a lattice. This technique has been extend to the coupled lattice [16] and implemented in LEGO.

**NONLINEAR ANALYSIS**

There are many different ways to compute lattice functions. Among them, the method outlined in the previous section is the simplest one to extend to the case when non-linearity is in presence. We start with a truncated Taylor map $M_n(z, \delta)$ that is extracted from a lattice by tracking a truncated power series of the order $n$ [8]. For simplicity, we assume that $\delta$ is the relative momentum and the RF cavities have been turned off so that $\delta$ is a constant of the motion. It has been shown [17] that one can construct perturbatively order-by-order a nonlinear transformation $A^{-1}(J, \psi, \delta)$ to find high-order invariance,

$$\mathcal{M}_n(J, \psi, \delta) = A^{-1}(J, \psi, \delta) e^{-H_{n+1}(J, \delta)}: \mathcal{A}(J, \psi, \delta),$$

(24)

where $J, \psi$ are the action-angle variables [10] and

$$\mathcal{A}(J, \psi, \delta) = e^{F_3(J, \psi, \delta)} \cdots e^{F_3(J, \psi, \delta)}: \mathcal{A}_1(J, \psi) \mathcal{A}_0(\delta).$$

(25)

Figure 4: Chromatic tune and beta as a function of relative momentum $\delta$ computed by two different methods.

We have the well-known result: $H_n(J, \delta) = 2\pi(\nu_x J_x + \nu_y J_y + \xi_x \delta J_x + \xi_y \delta J_y + \ldots)$, where $\xi_{x,y}$ are the chromaticities. Here, we would like to demonstrate that, from $\mathcal{A}(J, \psi, \delta)$, one can extract the closed dispersive orbit and chromatic lattice functions as polynomials of $\delta$. The formula for the chromatic Courant-Snyder parameters is identical to Eq. (22) except that all the matrix elements become polynomials of $\delta$. In particular, we have $\beta(\delta) = \tilde{A}_{11}^2(\delta) + \tilde{A}_{12}^2(\delta)$.

We calculate the chromatic tune and beta at the interaction point of the High Energy Ring in PEP-II using two different methods. Using LEGO, in the first approach, for a given $\delta$, we numerically search the closed orbit, extract a linear map relative to the closed orbit, and analyze the tune and beta function according to the linear analysis outlined in the previous section. In the second computation, we extract a 10th order Taylor map to make the normal form as outlined in this section to compute the tune and beta function as a polynomial of $\delta$ using LIELIB [17]. For a given
\( \delta \), we evaluate the polynomial at the end. The results of the two calculations are identical and are shown in Fig. 4. Similarly, the dispersive orbits obtained using the two different methods agree accurately.

The agreement between the two methods demonstrates one of the most important features of the symplectic-integrator based codes. That is intrinsically inherited consistency between the direct numerical calculation and the nonlinear analysis based on a very high-order transfer map. This feature gives us the confidence to use the map to identify the nonlinear aberrations that might cause the stability problem for the particles in circular accelerators.

Similar to the linear analysis, we can propagate the nonlinear \( \mathcal{A}(J, \psi, \delta) \) from \( s_1 \) to \( s_2 \) with

\[
\mathcal{A}(s_2) = \mathcal{A}(s_1) \mathcal{M}_{12},
\]

where \( \mathcal{M}_{12} \) is the nonlinear transfer map between \( s_1 \) and \( s_2 \). It is not hard to show that \( \mathcal{A}(s_2) \) also normalizes the coordinates at position \( s_2 \) because \( H(J, \delta) \) is also a global invariance. Once again, the chromatic lattice functions and phase advance can be extracted from \( \mathcal{A}(s_2) \).

**CONCLUSION**

In this paper, the codes based on canonical integrators are discussed and studied in detail ranging from the underlining principles to practical analysis. The integrators outlined in the paper are most suitable to be applied to compact and small circular accelerators where any approximations have to be carefully examined and justified.

We introduce canonical integrators as a method of tracking charged particles in a static magnetic field. In the process, we establish the TEAPOT algorithms as a second-order integrator in the Hamiltonian system. As a result, we make it applicable to accelerators that do not reside in the horizontal plane.

We give a method that uniformly treats both the linear and nonlinear analysis based on the normal form. Using the truncated power series and normal form analysis, we can compute the tune and beta function as polynomials of the momentum deviation \( \delta \) up to an arbitrary order. Moreover, the method is still applicable even when linear coupling is present. This technique is a general extension to HARMON [18] which is limited to the third order of \( \delta \). This method could become extremely useful and necessary when we design an even stronger final focusing system for the next generation colliders.

There are many challenging works to be pursued. Among them: what are most efficient and accurate integrators for the fringe field in small machines? What determines the stability of particle in the circular accelerators? How to determine the dynamic aperture without actually tracking particles?

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