Symplectic Mapping in Systems with Three-Dimensional Magnetic Fields

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A differential algebraic integration algorithm is developed for symplectic particle mapping through three-dimensional (3D) magnetic field configurations. The algorithm employs a canonical transformation to eliminate the linear part of the Hamiltonian. This is equivalent to solving the equations of motion with a Lorentz force for a reference orbit. The new Hamiltonian is then Taylor expanded around the reference orbit. Making thin slices along the longitudinal coordinate and using differential algebras, one can calculate and store the energy-dependent reference orbit, the coordinate-dependent vector potential, and thus the Hamiltonian as well as the symplectic map in a Lie transformation form at each slice. The section map from the entrance to the exit in the 3D magnetic field structure is then concatenated through the slices. This procedure can be used to obtain particle transfer maps for insertion devices, solenoids, fringe fields of dipoles and quadruples, and other complicated magnetic configurations.

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I. INTRODUCTION

Particle motion and the beam trajectory in most particle accelerators are usually well approximated using the dominant transverse magnetic fields. In this case, a single longitudinal component of the magnetic vector potential $A_s(s)$ is sufficient to describe the system, where the longitudinal coordinate $s$ is the time-like independent variable. The Hamiltonian, which governs the transverse particle motion in the Frenet-Serret coordinate system, can be separated into two terms, where one depends only on coordinates and the other on the momenta [1]. Therefore, the phase-space coordinates can be computed with the conventional symplectic integrators [2, 3] that handle the momenta and coordinates separately to a desired order.

In recent years, superconducting magnets and specially designed insertion devices (IDs), such as gap- and phase-adjustable elliptical-polarization undulators (EPUs), have been developed to generate polarized lights in high performance storage rings. The widely used undulators and wigglers can produce high-brightness lights in the third and future generation light sources, and can also be used to modify the emittance and the damping partition numbers for attaining high quality electron beams. In these devices, the magnetic field has a non-negligible, longitudinal component. The 3D magnetic field can no longer be represented by a single component of the vector potential. In a properly chosen gauge, a
vector potential with a minimum of two components can be used to describe such a system. In accelerator applications, the two transverse components, $A_x(s)$ and $A_y(s)$, are generally preferred. However, the corresponding Hamiltonian for particle motion cannot be separated into a term involving only momenta and a term involving only coordinates. Thus we cannot take advantage of the conventional symplectic integration methods. This paper is intended to study methods for solving this task.

In the past 20 years, there was a great effort in the development of particle tracking and the calculation of maps for complex accelerator beam lines. These treatments deal essentially with a 2D magnetic field that can be represented by a single vector potential component $A_z$. On the other hand, all previous methods used in the tracking of a 3D magnetic field are based on the paraxial approximation (see e.g. Ref. [4]). Since the reference orbit in a wiggler differs substantially from that of a fixed straight line orbit, the effect of feeddown from higher order multipoles is important. While it is possible to track particle motion based on the paraxial approximation and determine the dynamical aperture of the accelerator, the physical interpretation of the resulting higher order maps through this tracking method is less obvious.

On the other hand, our approach, extended from our previous work [5], involves the following key points.

1. Carry out a canonical transformation with a generating function to eliminate the linear part of the Hamiltonian and obtain a new Hamiltonian expanded around the reference particle’s orbit in regions involving a 3D magnetic field. This new Hamiltonian includes the feeddown effects of higher order multipoles. The solution of the reference orbit is equivalent to solving the equations of motion with the Lorentz force.

2. Divide a beam-line subsystem into $N$-slices along the longitudinal coordinate, such that we can trace the reference particle’s trajectory from the entry to the mid-point of a slice by a drift-kick procedure using the canonical equations of motion, and from the mid-point to the end-point by a kick-drift procedure. The Hamiltonian in each slice is represented by the Hamiltonian at the mid-point. Note that the number of slices $N$ is determined by a desired accuracy and an affordable computation time. The boundary condition between adjacent slices requires that the vector potential is continuous.

3. Employ the method of differential algebras [6, 7] to obtain the Taylor-expanded vector potential and the Hamiltonian with respect to the reference orbit, which is simultaneously solved through the drift-kick-kick-drift (DKKD) procedure (see Appendix A) between the boundaries and mid-point of each slice. The Taylor map, to a pre-chosen order, can be extracted through the slices.

4. Save the Taylor maps between entrance and exit, and between certain pre-marked points along the beam-line. These Taylor maps can be Lie transformed and used repeatedly to represent the beam line section, called the section-map. Integrable polynomials [8] can then be repeatedly used for symplectic tracking of particles through these beam-lines.
This paper is intended to show the applicability of this method, and use a few examples to show the validity of this method. We describe the algorithm in detail in Sec. II. In Sec. III, we demonstrate the applicability of the algorithm with a few well-known magnetic field structures. Application of the algorithm to insertion devices is given in Sec. IV. The conclusion and future applications are given in Sec. V.

II. METHOD AND ALGORITHM

The Hamiltonian in the Frenet-Serret coordinate system is given by

\[ K = -qA_x - \left( 1 + \frac{x}{\rho} \right) \left[ P_m^2 - (P_x - qA_x)^2 - (P_y - qA_y)^2 \right]^{1/2}, \]  

where \( P_x \) and \( P_y \) are the canonical conjugate momenta, \( P_m \) is the magnitude of the mechanical momentum of the particle, \( q \) is the charge of the particle, \( A_x, A_y, \) and \( A_s \) are components of the vector potential in the Frenet-Serret coordinate system, and \( \rho \) is the radius of curvature. Let \( P_{m0} \) be the magnitude of the mechanical momentum of a reference synchronous particle. We define the fractional momentum deviation as \( \delta = \frac{P_m - P_{m0}}{P_{m0}} \) and scale the canonical conjugate momenta as \( p_x, p_y = \frac{P_x, P_y}{P_{m0}}. \) The dimensionless Hamiltonian, \( H = \frac{K}{P_{m0}} \), becomes

\[ H = -a_s - \left( 1 + \frac{x}{\rho} \right) \left[ (1 + \delta)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 \right]^{1/2}, \]  

where \( a_{x,y,s} = \frac{qA_{x,y,s}}{P_{m0}} = \frac{A_{x,y,s}}{B_p} \) are components of the dimensionless vector potential.

In most cases, the magnetic field in accelerator structures can be well approximated by transverse components such that a single longitudinal component of the vector potential \( A_s \) is sufficient to describe the classical particle motion. Since \( A_x = A_y = 0, \) the mechanical momenta \( P_{mx} \) and \( P_{my} \) are equal to their corresponding canonical conjugate momenta, \( P_x \) and \( P_y. \) Using Hamilton’s equation, we obtain

\[ u' \equiv \frac{du}{ds} = \frac{\partial H}{\partial p_u} \approx p_{mu} = p_u, \]  

where \( u \) stands for \( x \) or \( y. \) However, in the region (beam-line) with 3D magnetic field \( p_u \) differs from \( p_{mu}, \) but the dimensionless mechanical momentum is still approximately equal to \( u'. \) With the above clarification, we now proceed to describe the algorithm.

Let \( z \) represent the transverse particle phase-space coordinates, i.e. \( z(s) \equiv (x, p_x, y, p_y) \) \( \dagger, \) the Hamiltonian can be simply represented by \( H(z, \delta). \) Such a Hamiltonian may not be analytically solvable, but it can always be solved numerically with differential algebra techniques, by Taylor expanding it around a properly-chosen reference orbit or a
periodic closed orbit in phase space [5]. This can be achieved by first making a canonical transformation with the generating function

\[ F_2 = (x - x_0)(p_X + px_0) + (y - y_0)(p_Y + py_0), \]

such that the linear part of the transformed Hamiltonian vanishes. Note that reference orbit depends on the particle momentum deviation \( \delta \), i.e. \( z_0(\delta) = (x_0(\delta), px_0(\delta), y_0(\delta), py_0(\delta))^\dagger \).

From the generating function, we obtain the conjugate phase space coordinates as

\[ X = x - x_0, \quad Y = y - y_0, \quad px = px + px_0, \quad py = py + py_0, \]

and the new Hamiltonian becomes

\[ \mathcal{H} = H + \frac{\partial F_2}{\partial s}. \]

The reference orbit \( z_0(\delta) \) is chosen such that the Taylor expanded linear order in phase-space coordinates of the new Hamiltonian vanishes, i.e.

\[ \mathcal{H} = \sum_{j=2}^{\infty} \mathcal{H}_j, \]

where \( \mathcal{H}_j \) stands for a homogeneous polynomial of degree \( j \) in canonically transformed phase-space coordinates.

The constraint that, after canonical transformation, \( \mathcal{H}_1 = 0 \) to all orders in \( \delta \) yields

\[ \frac{\partial F_2}{\partial s} + \nabla H(z_0) \cdot Z = 0 \quad \text{with} \quad Z \equiv (X, px, Y, py)^\dagger, \]

or

\[ \begin{align*}
\frac{\partial x_0}{\partial s} &= \frac{\partial H}{\partial px}, & \frac{\partial px_0}{\partial s} &= -\frac{\partial H}{\partial X}, \\
\frac{\partial y_0}{\partial s} &= \frac{\partial H}{\partial py}, & \frac{\partial py_0}{\partial s} &= -\frac{\partial H}{\partial Y}.
\end{align*} \]

For simplicity, we represent a general 3D magnetic field with two transverse vector potential components, i.e. \( a_s = 0 \). In the following, we will show that this reference orbit \( z_0 \) is actually the reference particle orbit that obeys the Lorentz force law. We consider a straight beam line section with \( 1/\rho = 0 \) to represent local Cartesian coordinates and use the non-relativistic expansion of the transverse Hamiltonian:

\[ H(x, px, y, py; s) \approx \frac{1}{2} [px - a_x]^2 + \frac{1}{2} [py - a_y]^2. \]

Equations (8) and (9) of the reference orbit become

\[ \begin{align*}
\frac{\partial x_0}{\partial s} &= \frac{\partial H}{\partial px} = px_0 - a_x(z_0), \\
\frac{\partial y_0}{\partial s} &= \frac{\partial H}{\partial py} = py_0 - a_y(z_0).
\end{align*} \]
\[ \frac{\partial p_{x_0}}{\partial s} = -\frac{\partial H}{\partial X} = \left\{ [p_{x_0} - a_x(z_0)] \frac{\partial a_x(z_0)}{\partial X} + [p_{y_0} - a_y(z_0)] \frac{\partial a_y(z_0)}{\partial X} \right\}, \quad (13) \]

\[ \frac{\partial p_{y_0}}{\partial s} = -\frac{\partial H}{\partial Y} = \left\{ [p_{x_0} - a_x(z_0)] \frac{\partial a_x(z_0)}{\partial Y} + [p_{y_0} - a_y(z_0)] \frac{\partial a_y(z_0)}{\partial Y} \right\}. \quad (14) \]

Thus the reference orbit \( z_0 \) obeys the equation of motion with the Lorentz force:

\[ \frac{d^2 x_0}{ds^2} = \frac{q}{p} \left[ B_s(z_0) \frac{dy_0}{ds} - B_y(z_0) \right]. \quad (15) \]

\[ \frac{d^2 y_0}{ds^2} = \frac{q}{p} \left[ B_x(z_0) - B_s(z_0) \frac{dx_0}{ds} \right]. \quad (16) \]

To avoid repeated calculations of the reference orbit for each particle with different energy, we calculate only once the reference orbit in a truncated Taylor expansion of \( \delta \). The dispersion function becomes

\[ d_0 = \left. \frac{dz_0}{d\delta} \right|_{\delta=0}. \quad (17) \]

To facilitate this numerical process, the longitudinal coordinate of a subsystem is divided into \( N \) slices. The reference orbit, the vector potential and the Hamiltonian are simultaneously obtained with differential algebras and recorded at the mid-points and the boundary points of the \( N \)-slices by solving the Hamilton equations (Eqs. (11)–(14)) as an initial value problem (see Appendix A for a DKKD procedure). This procedure includes all feed-down effects. The path difference between the reference orbit and the paraxial axis can provide information for RF frequency adjustment to compensate for the orbit distortion.

The Hamiltonian flow of the state vector \( Z \) can be advanced by using a Lie transformation as

\[ Z(s + \Delta s) = \exp \left\{ -\Delta s : \sum_{j=2}^{\infty} \mathcal{H}_j(\bar{s}) : \right\} \left. Z \right|_{Z=Z(s)} \quad (18) \]

in a slice of longitudinal length \( \Delta s \) with starting longitudinal coordinate \( s \) and mid-point longitudinal coordinate \( \bar{s} \). To save computer time, one need not advance the particle phase-space coordinates slice-by-slice. One would concatenate the Lie maps into one that represents the whole subsystem. To achieve this, one first represents the Lie map of the \( k \)-th slice, \([s_k, s_k + \Delta s]\), as

\[ \exp \left\{ -\Delta s : \sum_{j=2}^{\infty} \mathcal{H}_j(\bar{s}_k) : \right\} = \exp \{ : h_k + f_k : \} \]

where the linear part \( h_k \equiv -\Delta s \cdot \mathcal{H}_2(\bar{s}_k) \) and the nonlinear part \( f_k \equiv -\Delta s \cdot \sum_{j=3}^{\infty} \mathcal{H}_j(\bar{s}_k) \) can be separated by a symplectic integrator. Using the second order symplectic integrator, one obtains

\[ \exp \{ : h_k + f_k : \} = \exp \left\{ \frac{1}{2} h_k : \right\} \exp \{ : f_k : \} \exp \left\{ : \frac{1}{2} h_k : \right\}, \quad (19) \]
and the whole map as
\[
\mathcal{M} = \prod_{k=1}^{N} \left\{ e^{\frac{1}{2} h_k}; e^{f_k}; e^{\frac{1}{2} h_k} \right\} = e^{h}; e^{f}, \tag{20}
\]
where \(e^{h}\) is the concatenated linear map. The nonlinear map \(e^{f}\) can be evaluated by the method of integrable polynomials \([8]\). Therefore the initial state vector \(Z(s_i)\) at the entrance of a subsystem can be directly mapped to the final state vector \(Z(s_f)\) at the exit of the subsystem. One must keep in mind the continuity condition of mechanical momenta required at the entrance and the exit. If the transverse vector potentials are zero at both the entry \(s_i\) and the exit \(s_f\), then the transverse canonical momenta in the state vector will be equal to their corresponding mechanical momenta. Otherwise, one should make an additional transformation between mechanical momenta and canonical momenta at the entrance and the exit.

III. DEMONSTRATION EXAMPLES

In this section, a quadrupole and a solenoid are used to illustrate and check the validity of the algorithm. Using a MATLAB based TPSA toolbox \([9]\), we obtain the Lie maps with a two-component vector potential and compare them with the analytical result.

III-1. Quadrupole

The vector potential of a quadrupole field is usually conveniently represented by a single longitudinal component
\[
A \equiv (A_x, A_y, A_s) = \left( 0, 0, \frac{B_1}{2}(y^2 - x^2) \right),
\]
where \(B_1 = \frac{\partial B_y}{\partial x}\). To check our algorithm, it can also be represented by two transverse components:
\[
A = (B_1 xs, -B_1 ys, 0).
\]

We can carry out a canonical transformation with the generating function
\[
F_2 = (p_{mx} \cdot x + p_{my} \cdot y) - \frac{qB_1}{2B\rho}(y^2 - x^2)s.
\]
The conjugate phase space coordinates are then transformed as
\[
X = \frac{\partial F_2}{\partial p_{mx}} = x, \quad p_x = \frac{\partial F_2}{\partial x} = p_{mx} + a_x,
\]
\[
Y = \frac{\partial F_2}{\partial p_{my}} = y, \quad p_y = \frac{\partial F_2}{\partial y} = p_{my} + a_y,
\]
and the new Hamiltonian becomes
\[ H(X, p_{mx}, Y, p_{my}; s) = H + \frac{\partial F_2}{\partial s} = -\frac{q B_1}{2B_0} (Y^2 - X^2) + \left(1 + \delta \right)^2 - p_{mx}^2 - p_{my}^2 \right)^{1/2}. \]

This Hamiltonian is identical to that derived from the \( A_s \) vector potential.

Analytically, the Hill’s equation obtained by both of these two vector potential forms is identical. Thus we expect to obtain an identical transfer map, given by [10]
\[
M = \begin{pmatrix}
\cos(\sqrt{K}|L|) & \sin(\sqrt{K}|L|) & 0 & 0 \\
-\sqrt{K}\sin(\sqrt{K}|L|) & \cos(\sqrt{K}|L|) & 0 & 0 \\
0 & 0 & \cosh(\sqrt{K}|L|) & \sinh(\sqrt{K}|L|)/\sqrt{|K|} \\
0 & 0 & \sqrt{|K|}\sinh(\sqrt{K}|L|) & \cosh(\sqrt{K}|L|)
\end{pmatrix}.
\]

Verifying the above transfer matrix is straightforward for the conventional choice, which happens to have an \( s \)-independent vector potential. It would be of interest to verify the above result by the numerical process outlined in Sec. II. We consider an example of calculating the transfer matrix using the algorithm for a focusing quadrupole with focusing strength \( K = B_1/B_0 \rho = 2.870480 \ m^{-2} \) and length \( L = 0.35 \ m \), used in the 1.5 GeV electron \( q = -e \) storage ring with \( B_0 \rho = -5.00346 \ T \cdot m \) at the Taiwan Light Source.

Since the Hamiltonian has already no linear order, no canonical transformation is needed for finding the reference orbit. That is, the reference orbit is straight line passing through the center of quadrupole. We set the entry position \( s_i = 0 \) such that the particle’s mechanical momenta are the same as the canonical momenta. However, at the exit position, \( s_f = L^- \), an additional transformation has to be made for the transfer map from canonical momenta to mechanical momenta, for the canonical momenta at \( s = L^+ \). This is because a hard-edge quadrupole prevents us from making the vector potential continuous on both boundaries. If the fringe fields had been included to achieve vector potential continuity at both boundaries, the additional transformation would not be necessary. In Sec. IV, we can make the vector potential continuous along the reference orbit in modeling insertion devices by adjusting the constant term of each pole’s vector potential. Then the whole maps of insertion devices are obtained by a slice-by-slice symplectic integration directly without any additional transformation for the discontinuity of the vector potential.

The linear transfer matrix for a quadrupole in this case calculated with \( N = 20 \) longitudinal slices is given by
\[
M_{QF} = \begin{pmatrix}
0.8293 & 0.3299 & 0 & 0 \\
-0.9467 & 0.8293 & 0 & 0 \\
0 & 0 & 1.1810 & 0.3708 \\
0 & 0 & 1.0647 & 1.1810
\end{pmatrix},
\]
which agrees with the analytic matrix to better than \( 10^{-4} \). One may gain precision by taking higher order symplectic integrators and a larger number of slices. For the second order symplectic integrator, we find the deviation is proportional to \( 1/N^2 \).
III-2. Solenoid

A solenoid is a special component commonly used in a collider accelerator. Its single-longitudinal-component magnetic field \((B_x = 0, B_y = 0, B_s = b_0)\) can be represented by a vector potential given by

\[
A = \left( -\frac{b_0}{2}y, \frac{b_0}{2}x, 0 \right).
\]

Solving the coupled betatron equation of motion, one obtains the linear transfer matrix [10]

\[
M = \begin{pmatrix}
\cos^2 \theta & \sin \theta \cos \theta / g & \sin \theta \cos \theta & \sin^2 \theta / g \\
-g \sin \theta \cos \theta & \cos^2 \theta & -g \sin^2 \theta & \sin \theta \cos \theta \\
-\sin \theta \cos \theta & -\sin^2 \theta / g & \cos^2 \theta & \sin \theta \cos \theta / g \\
g \sin^2 \theta & -\sin \theta \cos \theta & -g \sin \theta \cos \theta & \cos^2 \theta
\end{pmatrix},
\]

where \(g = b_0/2B_0 \rho, \theta = gL\), and \(L\) is the solenoid length. Our algorithm for evaluating \(\prod_{k=1}^{N} e^{-\Delta s H(s_k)}\) agrees with the above. Since the Hamiltonian is independent of \(s\), the precision of the numerical evaluation is independent of the number of slices.

IV. MODELING INSERTION DEVICES

One of the most important applications of this algorithm is the study of particle beam dynamics in storage rings with insertion devices used in the third generation light sources. The vector potential for IDs is described in Appendix B. We consider an ideal insertion device with harmonic \(n = 1\) to illustrate the applicability of this method.

Let \(m_{ID}\) be the number of end-poles at each side of an ideal ID and \(n_{ID}\) be the number of full-poles. The total number of poles is \(2m_{ID} + n_{ID} \). In the design of IDs, the magnetic field strength of the end-poles are always varied so that the first and the second integrations of the magnetic field are both zero, e.g. for a planar insertion device:

\[
\int_{s_i}^{s_f} B_y(x_0, y_0, s) ds = 0 , \tag{21}
\]

\[
\int_{s_i}^{s_f} ds \int_{s_i}^{s_f} B_y(x_0, y_0, s) ds = 0 . \tag{22}
\]

This condition is equivalent to saying that there is no net angular and orbital displacements in passing through the insertion device.

The magnetic field of an ID for the first harmonic \((n = 1)\) is given by (see Appendix B)

\[
n_{ID} = \text{odd} : \quad \begin{cases} 
B_x = f_1(x, y) \cos (k_s s) , \\ 
B_y = g_1(x, y) \cos (k_s s) , \\ 
B_s = h_2(x, y) \sin (k_s s) ,
\end{cases} \tag{23}
\]
FIG. 1: The magnetic field configuration, $B_y(s)$, of an ideal W20 wiggler structure at NSRRC. Middle: The corresponding vector potential, $A_x$, used in the calculation of the ideal W20 case. Bottom: The reference particle’s trajectory in the ideal NSRRC W20 wiggler is calculated by solving the Hamiltonian equations with the 2nd-order symplectic integrator.

\[
\begin{align*}
  n_{ID} & = \text{even : } \\
  B_x & = f_2(x, y) \sin (k_s s) , \\
  B_y & = g_2(x, y) \sin (k_s s) , \\
  B_s & = h_1(x, y) \cos (k_s s) ,
\end{align*}
\]

where the center of the IDs is taken as the reference point $s = 0$. The functions $f_i$, $g_i$, and $h_i$ are obtained by requiring the magnetic fields to obey the Maxwell equations. Although an insertion device may include higher harmonics in the field expansion, the first harmonic expansion in Eqs. (23) and (24) gives all the essential features of electron beam motion and synchrotron radiation.

The maximum field strength at each pole along the center line of an ID is usually prescribed and measured. The fields of the end poles are adjusted to achieve zero total field integrals. For example, we model the planar wiggler W20 at the Taiwan Light Source (TLS) with the ratio of pole strengths $(1/4, -3/4, 1, -1, \cdots, -1, 1, -3/4, 1/4)$ along the center orbit. Here we have $m_{ID} = 2$ and $n_{ID} = 23$. These pole strengths are sufficient to attain the reference orbit $(x_0, x'_0, y_0, y'_0) = (0, 0, 0, 0)$ at both entrance and exit of a wiggler.

In modeling IDs, the constant terms of the end-pole’s vector potentials are adjustable to be continuous along the trajectory of the reference particle, and we divide each pole into $N$ slices, i.e., there are total $N(2m_{ID} + n_{ID})$ slices for an insertion device. Hence, at the
interface of the slices, the mechanical momenta and the corresponding canonical momenta of the reference particle are continuous. Also the vector potentials of the end-poles vanish at both the entrance and exit of an ID, i.e. $p_{u_0}(s_i) = p_{mu_0}(s_i)$ and $p_{u_0}(s_f) = p_{mu_0}(s_f)$ where $u$ stands for $x$ or $y$. This allows for the obtaining of the whole maps of insertion devices by a slice-by-slice symplectic integration directory.

Fig. 1 shows the magnetic field (top), vector potential (middle), and the reference orbit (bottom) for a W20-like ideal ID with $n_{ID} = 23$ and $m_{ID} = 2$. Parameters used in this calculation are: $q = -e$, $B_0\rho = 5.00346$ T-m, $B_w = 1.8287$ T, $k_s = 31.4159$ m$^{-1}$, $L = 2.7$ m. The corresponding magnetic fields are given by

$$\begin{align*}
B_x &= 0, \\
B_y &= -B_w \cosh (k_s y) \cos (k_s s), \\
B_s &= B_w \sinh (k_s y) \sin (k_s s).
\end{align*}$$

The linear focusing strength can be extracted from the quadratic part of the Hamiltonian. With this algorithm we obtain the focusing strength $K = 0.0600$ m$^{-2}$, which agrees well
FIG. 3: The chart of the DKKD procedure. For the $k$-th slice, after the reference particle’s parameterized phase-space coordinates are advanced by a drift-kick procedure with differential algebras, we obtain the time-explicitly-independent Hamiltonian at the mid-point. Then the reference particle’s coordinates are advanced by another kick-drift procedure to the exit of the $k$-th slice.

with the analytic formula:

$$K_{\text{eff}} = \left( \frac{B_w}{B_0 \rho} \right)^2 \langle \cos^2 (k_s s) \rangle = \left( \frac{B_w}{B_0 \rho} \right)^2 \langle \sin^2 (k_s s) \rangle = 0.5 \left( \frac{B_w}{B_0 \rho} \right)^2 .$$  \hspace{1cm} (25)

Similarly, we model the three-pole superconducting wavelength shifter (SWLS) at the TLS with a pole-strength ratio of $(1/2, -1, 1/2)$, which corresponds to $n_{\text{ID}} = 1$ and $m_{\text{ID}} = 1$. Fig. 2 shows the magnetic field (top), vector potential (middle), and the reference orbit (bottom) for the superconducting wavelength shifter (SWLS) with parameters $B_w = 5.9446$ T, $k_s = 15.7080 \text{ m}^{-1}$ and $L = 0.6 \text{ m}$. The reference particle orbit deviates from the center line by a substantial magnitude, which may cause a large path difference. The focusing strength extracted from the numerical algorithm is $K = 0.3550 \text{ m}^{-2}$, which again agrees with that of the analytic formula Eq. (25).

V. CONCLUSION AND DISCUSSION

We have developed a symplectic algorithm for particle tracking and mapping in a 3D magnetic field, where the vector potential cannot be described by $A_z$ alone.

We carry out a canonical transformation to solve the reference orbit in phase space by setting the linear order of the Taylor-expanded Hamiltonian to zero. Dividing a subsystem longitudinally into N-slices, we implement a drift-kick-kick-drift (DKKD) procedure to advance the reference orbit phase-space coordinates: (1) The reference orbit phase-space coordinates are advanced from the entrance of a slice by a drift-kick procedure to the mid-point where the Hamiltonian is recorded. (2) The reference orbit phase-space coordinates are further advanced to the exit by a kick-drift procedure. Each of these time-explicit-independent mid-point Hamiltonians represents the Hamiltonian for the corresponding slice. The advancement of phase-space coordinates with respect to the reference orbit are obtained by a Lie transformation. These Lie transformations can be concatenated into one for the subsystem. The transfer map can be evaluated by integrable polynomials.

The mechanical momenta must be continuous. This is automatically satisfied by imposing the continuity condition of the vector potential for insertion devices. To avoid
repeated calculation of a reference orbit for each particle with different energy, the reference orbit is actually Taylor expanded in the momentum deviation $\delta$. The dispersion function and the path length difference can be derived.

Since the Taylor expansion of the Hamiltonian maps is around the reference orbit, all feed-downs from higher-order multipoles are automatically included in the transfer map. We have successfully tested this algorithm using several examples including insertion devices.

For ring applications, one needs to recalculate the closed orbit of the entire accelerator. This method presented in this paper can be used to obtain the closed orbit. Since the resulting Hamiltonian is expanded around this closed orbit, the one-turn transfer map includes all feeddowns.

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APPENDIX A: A DIFFERENTIAL ALGEBRAIC DKKD PROCEDURE FOR OBTAINING THE REFERENCE TRAJECTORY AND THE TIME-EXPLICITLY-INDEPENDENT HAMILTONIANS

Suppose a 3D magnetic field is longitudinally located between $s_i$ and $s_f$ with $L = s_f - s_i$. We divide the subsystem into $N$-slices such that the length of each slice is $\Delta s = L/N$. The entry, mid-point, and exit of the $k$-th slice are $s_k = s_i + (k - 1)\Delta s$, $s_k = s_i + (k - 1/2)\Delta s$, and $s_{k+1} = s_i + k\Delta s$. The differential algebraic DKKD procedure for obtaining the parameterized reference particle’s trajectory and the associated Hamiltonian with respect to this to-be-obtained parameterized reference orbit in this slice is divided into the following steps. Note that this DKKD procedure only requires accuracy; it does not require symplecticity since the followed up tracking and mapping will be automatically symplectic once an accurate time-explicitly-independent Hamiltonian is obtained.

1. We evaluate the Hamiltonian $H(x, p_x, y, p_y, \delta; s_k)$, $dx/ds = \partial H/\partial p_x$ and $dy/ds = \partial H/\partial p_y$ at the slice-interface $s_k$. The coordinates of the reference orbit are advanced to the mid-point $\bar{s}_k$ by

$$x_0(\delta, \bar{s}_k) = x_0(\delta, s_k) + (\Delta s/2) \cdot \frac{\partial H}{\partial p_x} \bigg|_{x_0(\delta, s_k), p_{x_0}(\delta, s_k), y_0(\delta, s_k), p_{y_0}(\delta, s_k)},$$

$$y_0(\delta, \bar{s}_k) = y_0(\delta, s_k) + (\Delta s/2) \cdot \frac{\partial H}{\partial p_y} \bigg|_{x_0(\delta, s_k), p_{x_0}(\delta, s_k), y_0(\delta, s_k), p_{y_0}(\delta, s_k)}.$$
2. We now evaluate $H$ with the updated new reference coordinates, $dp_x/ds = -\partial H/\partial x$ and $dp_y/ds = -\partial H/\partial y$, at the mid-point of the slice. The conjugate momenta of the reference orbit at the mid-point are advanced by

$$p_{x_0}(\delta, \bar{s}_k) = p_{x_0}(\delta, s_k) - (\Delta s/2) \cdot \frac{\partial H}{\partial x} \bigg|_{x_0(\delta, \bar{s}_k), p_{x_0}(\delta, \bar{s}_k), y_0(\delta, \bar{s}_k), p_{y_0}(\delta, \bar{s}_k)} \quad \text{(A3)}$$

$$p_{y_0}(\delta, \bar{s}_k) = p_{y_0}(\delta, s_k) - (\Delta s/2) \cdot \frac{\partial H}{\partial y} \bigg|_{x_0(\delta, \bar{s}_k), p_{x_0}(\delta, \bar{s}_k), y_0(\delta, \bar{s}_k), p_{y_0}(\delta, \bar{s}_k)} \quad \text{(A4)}$$

3. The Hamiltonian $H(x, p_x, y, p_y; \delta; \bar{s}_k)$, $dp_x/ds = -\partial H/\partial x$, and $dp_y/ds = -\partial H/\partial y$ at the mid-point can be evaluated. Changing the conjugate phase-space coordinates $(X = x - x_0, p_X = p_x - p_{x_0}, Y = y - y_0, p_Y = p_y - p_{y_0})$ at the mid-point $\bar{s}_k$, one can evaluate and save the Hamiltonian, $H(\delta, \bar{s}_k) = h_k + f_k$, which describes the dynamics and is Taylor-expanded around the parameterized reference orbit. It is integrated with the previous concatenated map by a second-order symplectic integrator for obtaining the section-map.

4. With the $dp_x/ds = -\partial H/\partial x$ and $dp_y/ds = -\partial H/\partial y$ obtained at this mid-point, the conjugate momenta of the reference orbit are then advanced to the end-point $s_{k+1}$ of the $k$-th slice by

$$p_{x_0}(\delta, s_{k+1}) = p_{x_0}(\delta, \bar{s}_k) - (\Delta s/2) \cdot \frac{\partial H}{\partial x} \bigg|_{x_0(\delta, \bar{s}_k), p_{x_0}(\delta, \bar{s}_k), y_0(\delta, \bar{s}_k), p_{y_0}(\delta, \bar{s}_k)} \quad \text{(A5)}$$

$$p_{y_0}(\delta, s_{k+1}) = p_{y_0}(\delta, \bar{s}_k) - (\Delta s/2) \cdot \frac{\partial H}{\partial y} \bigg|_{x_0(\delta, \bar{s}_k), p_{x_0}(\delta, \bar{s}_k), y_0(\delta, \bar{s}_k), p_{y_0}(\delta, \bar{s}_k)} \quad \text{(A6)}$$

5. The $H$ at the mid-point is re-evaluated with the updated new reference momenta. The $dp_x/ds = -\partial H/\partial x$ and $dp_y/ds = -\partial H/\partial y$ are also obtained. The coordinates of the reference orbit are advanced to the end-point $s_{k+1}$ of the $k$-th slice by

$$x_0(\delta, s_{k+1}) = x_0(\delta, \bar{s}_k) + (\Delta s/2) \cdot \frac{\partial H}{\partial p_x} \bigg|_{x_0(\delta, \bar{s}_k), p_{x_0}(\delta, s_{k+1}), y_0(\delta, \bar{s}_k), p_{y_0}(\delta, s_{k+1})} \quad \text{(A7)}$$

$$y_0(\delta, s_{k+1}) = y_0(\delta, \bar{s}_k) + (\Delta s/2) \cdot \frac{\partial H}{\partial p_y} \bigg|_{x_0(\delta, \bar{s}_k), p_{x_0}(\delta, s_{k+1}), y_0(\delta, \bar{s}_k), p_{y_0}(\delta, s_{k+1})} \quad \text{(A8)}$$

Using conjugate phase-space coordinates at the end-point $s_{k+1}$, one evaluates the Hamiltonian $H(x, p_x, y, p_y; s_{k+1})$, $dp_x/ds = -\partial H/\partial x$, and $dp_y/ds = -\partial H/\partial y$. The integration procedure repeats for the next slice.
The DKKD procedure is schematically shown in Figure 3. In this integration algorithm, an important constraint is the continuity of the vector potential at the interface of each slice. The DKKD procedure need not be symplectic, similar to the traditional Runge-Kutta integration method. We carry out the DKKD integration only once for attaining an accurate reference orbit. The dependence of the reference orbit on $\delta$ is included up to a desired order and the resulting transfer map, given by $\exp\{-\Delta s : \mathcal{H}(\delta, \hat{s}_k) :\}$, is symplectic.

APPENDIX B: 3D MAGNETIC FIELD AND VECTOR POTENTIAL FOR INSERTION DEVICES

A general 3D magnetic field can be represented by a Fourier-Floquet expansion:

\[
B_x = \sum_{n=1}^{\infty} \left[ f_{1n}(x, y) \cos(nk_s s) + f_{2n}(x, y) \sin(nk_s s) \right] + f_0(x, y),
\]

\[
B_y = \sum_{n=1}^{\infty} \left[ g_{1n}(x, y) \cos(nk_s s) + g_{2n}(x, y) \sin(nk_s s) \right] + g_0(x, y),
\]

\[
B_z = \sum_{n=1}^{\infty} \left[ h_{1n}(x, y) \cos(nk_s s) + h_{2n}(x, y) \sin(nk_s s) \right] + h_0(x, y),
\]

where $(\hat{x}, \hat{y}, \hat{s})$ form the basis of the orthogonal coordinate system, $x$ and $y$ are the transverse position coordinates, $s$ is the longitudinal distance serving as the time-like variable, and $k_s = 2\pi/\lambda_s$ is the wave vector.

Using the Maxwell equations, $\nabla \cdot B = 0$ and $\nabla \times B = 0$, we find that the functions $f_0, g_0, h_0$ satisfy $\partial_x g_0 = \partial_y f_0$, $\partial_y g_0 + \partial_x f_0 = 0$, $h_0 = \text{constant}$, and the functions $f_{1n}, f_{2n}, g_{1n}, g_{2n}, h_{1n},$ and $h_{2n}$ are given by the following two sets:

\[
f_{1n} = -k_{2nx} (\alpha_{2n} s \sin 2n x + \beta_{2n} c \sin 2n x) (\gamma_{2n} s \sin 2n y + \delta_{2n} s \sin 2n y),
\]

\[
f_{2n} = k_{1nx} (\alpha_{1n} s \sin 1n x + \beta_{1n} c \sin 1n x) (\gamma_{1n} s \sin 1n y + \delta_{1n} s \sin 1n y),
\]

\[
g_{1n} = -k_{2ny} (\alpha_{2n} c \sin 2n x + \beta_{2n} s \sin 2n x) (\gamma_{2n} c \sin 2n y + \delta_{2n} s \sin 2n y),
\]

\[
g_{2n} = k_{1ny} (\alpha_{1n} c \sin 1n x + \beta_{1n} s \sin 1n x) (\gamma_{1n} c \sin 1n y + \delta_{1n} s \sin 1n y),
\]

\[
h_{1n} = k_s (\alpha_{1n} s \sin 1n x + \beta_{1n} s \sin 1n x) (\gamma_{1n} s \sin 1n y + \delta_{1n} s \sin 1n y),
\]

\[
h_{2n} = k_s (\alpha_{2n} c \sin 2n x + \beta_{2n} s \sin 2n x) (\gamma_{2n} c \sin 2n y + \delta_{2n} s \sin 2n y),
\]

or

\[
f_{1n} = \kappa_{2nx} (\alpha_{2n} s \sin 2n x - \beta_{2n} c \sin 2n x) (\gamma_{2n} s \sin 2n y + \delta_{2n} s \sin 2n y),
\]

\[
f_{2n} = \kappa_{1nx} (-\alpha_{1n} s \sin 1n x + \beta_{1n} c \sin 1n x) (\gamma_{1n} s \sin 1n y + \delta_{1n} s \sin 1n y),
\]

\[
g_{1n} = -k_{2ny} (\alpha_{2n} c \sin 2n x + \beta_{2n} s \sin 2n x) (\gamma_{2n} c \sin 2n y + \delta_{2n} s \sin 2n y),
\]

\[
g_{2n} = k_{1ny} (\alpha_{1n} c \sin 1n x + \beta_{1n} s \sin 1n x) (\gamma_{1n} c \sin 1n y + \delta_{1n} s \sin 1n y),
\]

\[
h_{1n} = k_s (\alpha_{1n} s \sin 1n x + \beta_{1n} s \sin 1n x) (\gamma_{1n} s \sin 1n y + \delta_{1n} s \sin 1n y),
\]

\[
h_{2n} = k_s (\alpha_{2n} c \sin 2n x + \beta_{2n} s \sin 2n x) (\gamma_{2n} c \sin 2n y + \delta_{2n} s \sin 2n y),
\]
\[ h_{2n} = k_s (\alpha_{2n} \text{cn}_{2nx} + \beta_{2n} \text{sn}_{2nx}) (\gamma_{2n} \text{ch}_{2ny} + \delta_{2n} \text{sh}_{2ny}) , \]

where \( \text{ch}_{mn u} \equiv \cosh (nk_{mn u} u) \), \( \text{sh}_{mn u} \equiv \sinh (nk_{mn u} u) \), \( \text{cn}_{mn x} \equiv \cos (n\kappa_{mn x} x) \), \( \text{sn}_{mn x} \equiv \sin (n\kappa_{mn x} x) \), \( (m = 1, 2) \), \( u \) stands for either \( x \) or \( y \), and \( k_{mn x}^2 + k_{mn y}^2 = k_s^2 \), \( \kappa_{mn x}^2 + \kappa_{mn y}^2 = k_{mn y}^2 \). The parameter set of \( k \)'s, \( \alpha \)'s, \( \beta \)'s, \( \gamma \)'s, and \( \delta \)'s are determined by the characteristics of the three dimensional magnetic field \([11]\).

From the relation \( B = \nabla \times A \) the gauge transformation shows that we have the freedom to choose \( A_x = 0 \) and use only the transverse components of the vector potentials \( A_x \) and \( A_y \) to represent arbitrary 3-D static magnetic fields, i.e.

\[ A_x = \sum_{n=1}^{\infty} \frac{1}{nk_s} \left[ g_1(x, y) \sin (nk_s s) - g_2(x, y) \cos (nk_s s) \right] + g_0(x, y) s + G(x, y) , \tag{B2} \]

\[ A_y = \sum_{n=1}^{\infty} \frac{1}{nk_s} \left[ f_1(x, y) \sin (nk_s s) - f_2(x, y) \cos (nk_s s) \right] + f_0(x, y) s + F(x, y) , \tag{B3} \]

where \( \partial_x F(x, y) - \partial_y G(x, y) = h_0 \) and \( \partial_x f_0 = \partial_y g_0 \). Combined with the \( \partial_x f_0 + \partial_y g_0 = 0 \) and the \( \partial_x g_0 = \partial_y f_0 \) obtained above, we have \( f_0 = a_0 y \) and \( g_0 = a_0 x \), where \( a_0 \) is a constant.

References

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[1] There is a cross-term in a describing the curvilinear coordinate system in a dipole. However, one can treat the particle motion in a dipole analytically, the curvature term can be handled without approximation.