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A General Method for Symplectic Particle Tracking in a Three-dimensional Magnetic Field

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Abstract

A general method is presented for symplectic integration of particle orbit in a 3-dimensional magnetic field. The reference orbit in phase space is solved by eliminating the linear part of the Hamiltonian. The Hamiltonian flow can be obtained by the Lie algebraic techniques such as matrix maps for linear motion and integrable polynomials for nonlinear motion. Our method eases the difficult task of particle tracking through insertion devices with complex magnetic field configuration such as the elliptical-polarization undulator. It can also be applied to calculate the particle orbit through a dipole or a quadrupole to include the fringe field effects accurately.

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Insertion devices (IDs) such as undulators and wigglers are widely used in high performance storage rings. They 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 recent years, specially designed IDs, such as gap- and phase-adjustable Elliptical-Polarization Undulators (EPUs), have been developed to generate polarized lights. Because of the complex magnetic field configurations in EPUs, it is difficult to obtain accurate maps for particle tracking. Since dynamical aperture depends sensitively on IDs with nonlinear magnetic field, it is important to find a nonlinear map for these devices.

For accelerators, the magnetic field configuration treated in the past can usually be described by a two-dimensional transverse magnetic field model. In this model, only the longitudinal component of the vector potential is needed to describe the system. Since the coordinates and their conjugate canonical momenta are not mixed in the Hamiltonian, the particle motion can easily be handled in the tracking programs. Since the fringe field or the magnetic field in an EPU is three-dimensional, the vector potential can not be solely described by a longitudinal component. A new algorithm is needed to handle this complicated magnetic field configuration.

In the past, there are several symplectic schemes proposed to solve particle tracking problems for complex wigglers. However, some of these methods neither solve the "true" reference orbit nor take advantage of the symplectic integrators [1]. On the other hand, the straight forward particle tracking in the straight rectangular coordinate system proposed in Ref. [2] may cause a mixed reference orbit and true betatron coordinates. This paper studies a general algorithm of solving a Hamiltonian system for a complex magnetic field configuration. The reference orbit is obtained through a canonical transformation that eliminates linear terms. Particle tracking can then be carried out by symplectic integrators and integrable polynomials.

Because of the periodic nature of IDs, the three-dimensional magnetic field can be presented by a Fourier-Floquet expansion:

$$
\begin{aligned}
B_x &= \sum_{n=1}^{\infty}\Big[f_{1n}(x,y)\cos(nk_s s) + f_{2n}(x,y)\sin(nk_s s)\Big] + f_0(x,y)\\
B_y &= \sum_{n=1}^{\infty}\Big[g_{1n}(x,y)\cos(nk_s s) + g_{2n}(x,y)\sin(nk_s s)\Big] + g_0(x,y)\\
B_s &= \sum_{n=1}^{\infty}\Big[h_{1n}(x,y)\cos(nk_s s) + h_{2n}(x,y)\sin(nk_s s)\Big] + h_0(x,y),
\end{aligned}
\tag{1}
$$

where $(\hat{x}, \hat{y}, \hat{s})$ forms 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, the functions f_0, g_0, h_0 satisfy $\partial_x g_0 = \partial_y f_0$, $\partial_y g_0 = \partial_x f_0$, and $h_0 =$ constant, $k_s = 2\pi/\lambda_s$ is the wave vector, and the functions f_{1n}, f_{2n}, g_{1n}, g_{2n}, h_{1n}, and h_{2n} are obtained from Maxwell's equations $\nabla \cdot \mathbf{B} = 0$ and $\nabla \times \mathbf{B} = 0$. Thus we have

$$
\begin{aligned}
f_{1n} &= -k_{2nx}\left(\alpha_{2n}s_{2nx} + \beta_{2n}c_{2nx}\right)\left(\gamma_{2n}c_{2ny} + \delta_{2n}s_{2ny}\right),\\
f_{2n} &= k_{1nx}\left(\alpha_{1n}s_{1nx} + \beta_{1n}c_{1nx}\right)\left(\gamma_{1n}c_{1ny} + \delta_{1n}s_{1ny}\right),\\
g_{1n} &= -k_{2ny}\left(\alpha_{2n}c_{2nx} + \beta_{2n}s_{2nx}\right)\left(\gamma_{2n}s_{2ny} + \delta_{2n}c_{2ny}\right),\\
g_{2n} &= k_{1ny}\left(\alpha_{1n}c_{1nx} + \beta_{1n}s_{1nx}\right)\left(\gamma_{1n}s_{1ny} + \delta_{1n}c_{1ny}\right),\\
h_{1n} &= k_s\left(\alpha_{1n}c_{1nx} + \beta_{1n}s_{1nx}\right)\left(\gamma_{1n}c_{1ny} + \delta_{1n}s_{1ny}\right),\\
h_{2n} &= k_s\left(\alpha_{2n}c_{2nx} + \beta_{2n}s_{2nx}\right)\left(\gamma_{2n}c_{2ny} + \delta_{2n}s_{2ny}\right),
\end{aligned}
$$

where u stands for either x or y, $c_{mnu} \equiv \cosh(nk_{mnu}u)$, $s_{mnu} \equiv \sinh(nk_{mnu}u)$, $(m = 1, 2)$, and $k_{mnx}^2 + k_{mny}^2 = k_s^2$. The parameter set of k's, α's, β's, γ's, and δ's are determined by the characteristics of the three dimensional magnetic field [3]. From the relation, $\mathbf{B} = \nabla \times \mathbf{A}$, we can choose $A_s = 0$ and find A_x and A_y as:

$$
A_x = \sum_{n=1}^{\infty}\frac{1}{nk_s}\Big[g_{1n}(x,y)\sin(nk_s s) - g_{2n}(x,y)\cos(nk_s s)\Big] + g_0(x,y)s + G(x,y), \tag{2}
$$

$$
A_y = \sum_{n=1}^{\infty}\frac{-1}{nk_s}\Big[f_{1n}(x,y)\sin(nk_s s) - f_{2n}(x,y)\sin(nk_s s)\Big] + f_0(x,y)s + F(x,y), \tag{3}
$$

where $\partial_x F(x,y) - \partial_y G(x,y) = h_0$.

The Hamiltonian in Frenet-Serret coordinate system is [4, 5]

$$
H = \frac{-e}{c}A_s - \left(1 + \frac{x}{\rho}\right)p\left[1 - \left(\frac{P_x}{p} - \frac{eA_x}{cp}\right)^2 - \left(\frac{P_y}{p} - \frac{eA_y}{cp}\right)^2\right]^{1/2}, \tag{4}
$$

where P_x and P_y are the canonical momenta, p is the magnitude of the mechanical momentum of the particle, and ρ is the radius of curvature. For the 3-dimensional magnetic field discussed above, we choose $A_s = 0$ and $1/\rho = 0$. Since p is much larger than the transverse mechanical momenta, $p_x = P_x - \frac{e}{c}A_x$ and $p_x = P_y - \frac{e}{c}A_y$, the particle Hamiltonian can be approximated by

$$H\left(x, P_x, y, P_y; s\right) \simeq \frac{1}{2p}\left[P_x - \frac{e}{c}A_x\right]^2 + \frac{1}{2p}\left[P_y - \frac{e}{c}A_y\right]^2. \tag{5}$$

Using Hamilton's equations, we obtain the equations of motion as

$$\frac{d^2x}{ds^2} = \frac{d}{ds}\left[\frac{P_x - (e/c)A_x}{p}\right] = \frac{e}{cp}\left(B_s\frac{dy}{ds} - B_y\right) \tag{6}$$

$$\frac{d^2y}{ds^2} = \frac{d}{ds}\left[\frac{P_y - (e/c)A_y}{p}\right] = \frac{e}{cp}\left(B_x - B_s\frac{dx}{ds}\right), \tag{7}$$

which states explicitly the transverse Lorentz force. In the following, we will describe our algorithm in solving the Lie generator for particle tracking in this type of undulators.

Let $\vec{z}$ represent the particle phase-space state vector, i.e. $\vec{z}(s) \equiv (x, P_x, y, P_y)^{\dagger}$. The Hamiltonian flow can be best described by expanding the Hamiltonian around a reference orbit, where the linear part of the Hamiltonian is transformed away. To reach this goal, we consider the generating function:

$$F_2 = (x - x_0)(P_X + P_{x0}) + (y - y_0)(P_Y + P_{y0}), \tag{8}$$

where $\vec{z_0} = (x_0, P_{x_0}, y_0, P_{y_0})^{\dagger}$ is the reference orbit. From the generating function, we obtain $X = x - x_0, Y = y - y_0, P_x = P_X + P_{x_0}, P_y = P_Y + P_{y_0}$. The new Hamiltonian becomes

$$\mathcal{H} = H + \frac{\partial F_2}{\partial s}. \tag{9}$$

The reference orbit $\vec{z_0}$ is chosen such that the linear part in the expansion of the new Hamiltonian in the phase space coordinates vanishes, i.e. the new Hamiltonian in Taylor series becomes

$$\mathcal{H} = \sum_{i=2}^{\infty} \mathcal{H}_i, \tag{10}$$

where $\mathcal{H}_i$ stands for a homogeneous polynomial of degree i in canonical phase space coordinates, the constant term $\mathcal{H}_0$ is ignored and we have set $\mathcal{H}_1 = 0$. This constraint gives

$$\frac{\partial x_0}{\partial s} = \frac{P_{x_0} - (e/c)A_x(\vec{z}_0)}{p}, \tag{11}$$

$$\frac{\partial y_0}{\partial s} = \frac{P_{y_0} - (e/c)A_y(\vec{z}_0)}{p}, \tag{12}$$

$$\frac{\partial P_{x_0}}{\partial s} = \frac{e}{pc}\left\{\left[P_{x_0} - (e/c)A_x(\vec{z}_0)\right]\partial_x A_x(\vec{z}_0) + \left[P_{y_0} - (e/c)A_y(\vec{z}_0)\right]\partial_x A_y(\vec{z}_0)\right\}, \tag{13}$$

$$\frac{\partial P_{y_0}}{\partial s} = \frac{e}{pc}\left\{\left[P_{x_0} - (e/c)A_x(\vec{z}_0)\right]\partial_y A_x(\vec{z}_0) + \left[P_{y_0} - (e/c)A_y(\vec{z}_0)\right]\partial_y A_y(\vec{z}_0)\right\}. \tag{14}$$

These equations can be used to solve the reference orbit $\vec{z}_0$ that obeys the Lorentz force law, i.e.

$$\frac{d^2 x_0}{ds^2} = \frac{e}{pc}\left[B_s(\vec{z}_0)\frac{dy_0}{ds} - B_y(\vec{z}_0)\right], \tag{15}$$

$$\frac{d^2 y_0}{ds^2} = \frac{e}{pc}\left[B_x(\vec{z}_0) - B_s(\vec{z}_0)\frac{dx_0}{ds}\right]. \tag{16}$$

Note here that $\vec{z}_0$ is also a function of the momentum p. The dispersion vector evaluated at momentum p_0 is given by

$$\vec{d} = p_0 \left.\frac{d\vec{z}_0}{dp}\right|_{p=p_0}, \tag{17}$$

where p_0 is the momentum of a reference synchronous particle.

Once the reference orbit is found, all the coefficients of the new Hamiltonian in terms of Taylor series expansion given by Eq. (10) are determined. The symplectic Hamiltonian flow of the state vector $\vec{Z} \equiv (X, P_X, Y, P_Y)^\dagger$, can be expressed in Lie algebra as

$$\frac{d\vec{Z}}{ds} = \lim_{\Delta s \to 0} \frac{\exp\{-\Delta s : \mathcal{H} :\} - 1}{\Delta s}\vec{Z} = -\left[\mathcal{H}, \vec{Z}\right]. \tag{18}$$

This algorithm can be accurately and easily implemented by splitting an ID into small segments in the Lie transformation as

$$\vec{Z}(s + \Delta s) = \exp\left\{-\Delta s : \sum_{i=2}\mathcal{H}_i(\bar{s}) :\right\}\vec{Z}(s) \qquad \text{where} \quad \bar{s} \in [s, s + \Delta s] \tag{19}$$

to preserve the symplectic integration.

The second order part $\mathcal{H}_2$ and higher order part of the Hamiltonian can then be separately treated by symplectic integrator techniques [6]. For example, using the second order symplectic integrator, we obtain, in terms of Lie generators [7]

$$\exp\left\{:\sum_{i=2}\mathcal{H}_i:\right\} = \exp\left\{:\frac{1}{2}\mathcal{H}_2:\right\}\exp\left\{:\sum_{i=3}\mathcal{H}_i:\right\}\exp\left\{:\frac{1}{2}\mathcal{H}_2:\right\}. \tag{20}$$

Where the nonlinear Lie generator $\exp\left\{:\sum_{i=3}\mathcal{H}_i:\right\}$ can be solved with explicit integrable polynomial [8].

The canonical transformation to eliminate the $\mathcal{H}_1$ is equivalent to first locating the reference orbit $\vec{z}_0(s)$ and then transferring the coordinates (x, y) in the Cartesian frame to a new set of coordinates (X, Y) in the reference orbit frame. In general, the reference orbit cannot be obtained analytically and so a numerical solution is needed. To avoid repeated calculation of the reference orbit for each particle with different energy, we calculate only once the reference orbit in truncated Taylor expansion of $\delta \equiv \Delta p/p_0$, where $\Delta p = p - p_0$. The first-order coefficients of the expansion is the dispersion function given in Eq. (17). Note that the accuracy of the reference orbit calculation has nothing to do with symplecticity, that is, even if the reference orbit is not exactly calculated up to the computer machine precision, the process does not violet the symplectic condition. The coefficients of the transformed Hamiltonian and the Lie generators are also parameterized in truncated Taylor series. Because the reference orbit is solved by the canonical transformation of Hamilton's equations, feed-down effects from higher-order multi-poles are automatically included.

In summary, we have developed a method to track particle motion in a 3-dimensional magnetic field that can be represented by A_x and A_y. This method can be applied to analyze nonlinear beam dynamics and generates accurate maps for insertion devices with complicated magnetic field such as the EPU insertion devices, the fringe field of bending magnets, and the super-conducting wavelength shifter.

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