# Canonical Particle Tracking in Undulator Fields 

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## I. Abstract

A new algebraic mapping routine for particle tracking across wiggler and undulator fields is presented. It is based on a power series expansion of the generating function to guarantee fully canonical transformations. This method is 10 to 100 times faster than integration routines, applied in tracking codes like BETA or RACETRACK. The tracking method presented is not restricted to wigglers and undulators, it can be applied to other magnetic fields as well such as fringing fields of quadrupoles or dipoles if the suggested expansion converges.

## II. Taylor Expanded Particle Motion

The particle motion in the magnetic field is described by applying a map over a finite step length $z$. The map is Taylor expanded with respect to the two transverse angle variables $\left(x_{i}^{\prime}, y_{i}^{\prime}\right)$ at the starting point of the transformation and a third variable $x_{3}$, which is proportional to the inverse of the bending radius of the particle orbit taken at an appropriate reference point. This set of three expansion variables is unusual but fully sufficient for large bending radii and more efficient than the more commonly applied expansion with respect to the four transversal coordinates, two angle and two position variables.

As an example and to demonstrate the method we present here results of an expansion up to second order, results up to third order are available from the authors [1].

## The Mapping Routine

We start with a general form of the expansion for the particle motion:

$$
\begin{array}{rr}
x_{f} & =x_{i}+z x_{i}^{\prime}+\left(a_{0}+a_{1} x_{i}^{\prime}+a_{2} y_{i}^{\prime}+a_{3} \boldsymbol{x}_{3}\right) \boldsymbol{x}_{3} \\
x_{f}^{\prime} & = \\
x_{i}^{\prime}+\left(a_{0}^{\prime}+a_{1}^{\prime} x_{i}^{\prime}+a_{2}^{\prime} y_{i}^{\prime}+a_{3}^{\prime} \boldsymbol{x}_{3}\right) \boldsymbol{x}_{3} \\
y_{f} & =y_{i}+z y_{i}^{\prime}+\left(b_{0}+b_{1} x_{i}^{\prime}+b_{2} y_{i}^{\prime}+b_{3} \boldsymbol{x}_{3}\right) \boldsymbol{x}_{3} \\
y_{f}^{\prime}= & y_{i}^{\prime}+\left(b_{0}^{\prime}+b_{1}^{\prime} \boldsymbol{x}_{i}^{\prime}+b_{2}^{\prime} y_{i}^{\prime}+b_{3}^{\prime} \boldsymbol{x}_{3}\right) \boldsymbol{x}_{3},
\end{array}
$$

where the derivative with respect to the longitudinale coordinate $z$ is indicated by a prime; the inital and final transverse particle position ( $x$ and $y$ ) is indicated by an index ( $i$ and $f$ resp.). The coefficents $a_{i}$ and $b_{i}$ are dependent on the position coordinates at the starting point, on the
longitudinal step width $z$ and on the geometric shape $S$ of the magnetic field.

Inserting these expansions into the equations of motion, given in a fixed, cartesian coordinate system [2] $\left(W=\sqrt{1+x^{\prime 2}+y^{\prime 2}}\right):$

$$
\begin{aligned}
x^{\prime \prime} & =\frac{1}{(B \rho)_{0}} W\left[y^{\prime} B_{z}-\left(1+x^{\prime 2}\right) B_{y}+x^{\prime} y^{\prime} B_{x}\right] \\
y^{\prime \prime} & =\frac{-1}{(B \rho)_{0}} W\left[x^{\prime} B_{z}-\left(1+y^{\prime 2}\right) B_{x}+x^{\prime} y^{\prime} B_{y}\right]
\end{aligned}
$$

we obtain a recursion formula for the $a_{i}$ and $b_{i}$ coefficents with the result:

$$
\begin{aligned}
& a_{0}=-\int_{0}^{z} \int_{0}^{z} S_{i y} d z d z \\
& a_{1}=-\int_{0}^{z} \int_{0}^{z} z S_{i x y} d z d z \\
& a_{2}=+\int_{0}^{z} \int_{0}^{z}\left(S_{i z}-z S_{i y y}\right) d z d z \\
& a_{3}=+\int_{0}^{z} \int_{0}^{z}\left\{S_{i z} \int_{0}^{z} S_{i x} d z\right. \\
&-S_{i y y} \int_{0}^{z} \int_{0}^{z} S_{i x} d z d z \\
&\left.b_{0}=+\int_{0}^{z} \int_{0}^{z} S_{i x y} d z d z \int_{0}^{z} \int_{0}^{z} S_{i y} d z d z\right\} d z d z \\
& b_{1}=--\int_{0}^{z} \int_{0}^{z}\left(S_{i z}-z S_{i x x}\right) d z d z \\
& b_{3}=+\int_{0}^{z} \int_{0}^{z}\left\{S_{i z} \int_{0}^{z} S_{i y} d z\right. \\
&-S_{i x x} \int_{0}^{z} \int_{0}^{z} S_{i y} d z d z \\
&\left.+S_{i x y} \int_{0}^{z} \int_{0}^{z} S_{i x} d z d z\right\} d z d z,
\end{aligned}
$$

and $b_{2}=-a_{1}$. The function $S(x, y, z)$, the magnetic scalar potential $V_{p o t}(x, y, z)$ and the magnetic rigidity of the particle $(B \rho)_{0}$ are connected by the relation:

$$
S(x, y, z)=-V_{p o t} /\left(x_{3}(B \rho)_{0}\right)
$$

If we choose $x_{3}=1 / \rho_{0}$ as the inverse of the bending radius (or scaled to become dimensionless ) at a fixed reference point, all derivatives of $S(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ are defined and are indicated by an index. The function $S_{i}=S_{i}\left(x_{i}, y_{i}, z\right)$ and its derivatives are taken at the initial transversal particle position $\boldsymbol{x}_{\boldsymbol{i}}$ and $y_{i}$.

The transformation:

$$
\left(x_{i}, x_{i}^{\prime}, y_{i}, y_{i}^{\prime}\right) \Longrightarrow\left(x_{f}, x_{f}^{\prime}, y_{f}, y_{f}^{\prime}\right)
$$

is now well defined and these four equations form a second order map between the inital and final particle coordinates over a finite step length $z$.

## The Generating Function

To construct a generating function ( $G . F$.) from the transfer map we change the particle coordinates ( $x, x^{\prime}, y, y^{\prime}$ ) into canonical variables ( $q x, p x, q y, p y$ ). Up to second order we just rewrite: $q x=x, p x=x^{\prime}, q y=y, p y=y^{\prime}$. The transverse vector potential is asumed to be zero here, but it can be taken into account. In case of the periodic undulator field we easily find longitudinal positions were the transverse vector potential vanishes.

Rearranging the transfer map and expanding the result again we obtain an implicit transformation of the type:

$$
\left(q x_{i}, p x_{f}, q y_{i}, p y_{f}\right) \quad \Longrightarrow \quad\left(q x_{f}, p x_{i}, q y_{f}, p y_{i}\right)
$$

With the abbreviation $\tilde{a}_{i}=\left(a_{i}-z a_{i}^{\prime}\right) x_{3}$ and similarly for $\tilde{b}_{i}$ we find:

$$
\begin{aligned}
q x_{f}= & q x_{i}+p x_{f}\left(z+\tilde{a}_{1}\right)+p y_{f} \tilde{a}_{2}+\tilde{a}_{0} \\
& +\left(\tilde{a}_{3}-a_{0}^{\prime} \tilde{a}_{1}-b_{0}^{\prime} \tilde{a}_{2}\right) x_{3} \\
q y_{f}= & q y_{i}+p y_{f}\left(z+\tilde{b}_{2}\right)+p x_{f} \tilde{b}_{1}+\tilde{b}_{0} \\
& +\left(\tilde{b}_{3}-a_{0}^{\prime} \tilde{b}_{1}-b_{0}^{\prime} \tilde{b}_{2}\right) x_{3} \\
p x_{i}= & p x_{f}\left(1-a_{1}^{\prime} x_{3}\right)-p y_{f} a_{2}^{\prime} x_{3} \\
& -a_{0}^{\prime} x_{3}+\left(a_{0}^{\prime} a_{1}^{\prime}+b_{0}^{\prime} a_{2}^{\prime}-a_{3}^{\prime}\right) x_{3}^{2} \\
p y_{i}= & p y_{f}\left(1-b_{2}^{\prime} x_{3}\right)-p x_{f} b_{1}^{\prime} x_{3} \\
& -b_{0}^{\prime} x_{3}+\left(a_{0}^{\prime} b_{1}^{\prime}+b_{0}^{\prime} b_{2}^{\prime}-b_{3}^{\prime}\right) x_{3}^{2} .
\end{aligned}
$$

By adding appropriate correction terms these four equations can be identified with the partial derivatives of a G.F. $F=F\left(q x_{i}, p x_{f}, q y_{i}, p y_{f}\right)$ :

$$
\begin{array}{rlrl}
q x_{f} & \equiv \partial F / \partial p x_{f} & p x_{i} \equiv \partial F / \partial q x_{i} \\
q y_{f} \equiv \partial F / \partial p y_{f} & p y_{i} \equiv \partial F / \partial q y_{i}
\end{array}
$$

For the G.F. we choose an expansion:

$$
\begin{aligned}
F= & F_{00}+F_{10} p x_{f}+F_{01} p y_{f} \\
& +F_{20} p x_{f}^{2}+F_{11} p x_{f} p y_{f}+F_{02} p y_{f}^{2}
\end{aligned}
$$

Comparing the coefficents we obtain for the $F_{i j}$ :

$$
\begin{aligned}
& F_{10}=q x_{i}+\tilde{a}_{0}+\left(\tilde{a}_{3}-a_{0}^{\prime} \tilde{a}_{1}-b_{0}^{\prime} \tilde{a}_{2}\right) x_{3} \\
& F_{01}=q y_{i}+\tilde{b}_{0}+\left(\tilde{b}_{3}-a_{0}^{\prime} \tilde{b}_{1}-b_{0}^{\prime} \tilde{b}_{2}\right) x_{3} \\
& F_{11}=\tilde{a}_{2}\left(\equiv \tilde{b}_{1}\right) \\
& F_{20}=\left(z+\tilde{a}_{1}\right) / 2 \\
& F_{02}=\left(z+\tilde{b}_{2}\right) / 2
\end{aligned}
$$

and $F_{00}$ has to satisfy the two partial derivatives:

$$
\begin{aligned}
& \partial F_{00} / \partial q x_{i}=-a_{0}^{\prime} x_{3}+\left(a_{0}^{\prime} a_{1}^{\prime}+b_{0}^{\prime} a_{2}^{\prime}-a_{3}^{\prime}\right) x_{3}^{2} \\
& \partial F_{00} / \partial q y_{i}=-b_{0}^{\prime} x_{3}+\left(a_{0}^{\prime} b_{1}^{\prime}+b_{0}^{\prime} b_{2}^{\prime}-b_{3}^{\prime}\right) x_{3}^{2}
\end{aligned}
$$

This is the expanded form of a G.F. for arbitrary magnetic fields.

## III. Application to Undulator Fields

Now we apply the results of the last sections to an explicit description of the undulator field, by taking the formula for the magnetic scalar potential of an undulator as suggested by [3]:

$$
V_{p o t}=-\left(B_{0} / k_{z}\right) \cos \left(k_{x} x\right) \sinh \left(k_{y} y\right) \cos \left(k_{z} z\right),
$$

with $k_{z}^{2}+k_{x}^{2}=k_{y}^{2}$. We are able to present the G.F. for this field dependence; however, this function still contains a closed orbit offset. We define the closed orbit to be the periodic solution with coordinate values $p x_{i}=p x_{f}=0$, $q x_{i}=q x_{f}=1 /\left(k_{z}^{2} \rho_{m i n}\right)$, which repeats after one period and $\rho_{\min }$ is taken at maximum field in the midplane. We subtract this offset by a coordinate transformation and obtain a G.F. which describes the nonlinear particle transformation with respect to the closed orbit. Introducing the abbreviations $c x=\cos \left(k_{x} q x_{i}\right), s x=\sin \left(k_{x} q x_{i}\right)$, $c y=\cosh \left(k_{y} q y_{i}\right)$ and $s y=\sinh \left(k_{y} q y_{i}\right)$ we obtain the coefficients $F_{i j}$ :

$$
\begin{aligned}
& F_{00}=z x_{3}^{2}\left(k_{y}^{2} c x^{2} c y^{2}+k_{x}^{2} s x^{2} s y^{2}\right) /\left(2 k_{y}\right)^{2} \\
& F_{10}=q x_{i}-1 / 4 z^{2} x_{3}^{2} k_{x} s x c x\left(k_{x}^{2} c y^{2}+k_{x}^{2}\right) / k_{y}^{2} \\
& F_{01}=q y_{i}+1 / 4 z^{2} x_{3}^{2} k_{y} s y c y\left(k_{x}^{2} c x^{2}+k_{x}^{2}\right) / k_{y}^{2} \\
& F_{11}=z x_{3} c x s y\left(k_{y}^{2}+k_{x}^{2}\right) /\left(k_{z} k_{y}\right) \\
& F_{20}=z / 2-z x_{3} k_{x} s x c y / k_{z} \\
& F_{02}=z / 2+z x_{3} k_{x} s x c y / k_{z} .
\end{aligned}
$$

In this expansion we apply $x_{3}=1 /\left(k_{z} \rho_{\text {min }}\right)$. The step length $z$ is adjusted to integer multiples of the period length to simplify the integration over $z$. This is an exact solution up to second order plus some correction terms of third order.

If we consider only second order terms an averaged Hamiltonian can be found from the G.F.:

$$
F=F_{00}+q x_{i} p x_{f}+q y_{i} p y_{f}+z\left(p x_{f}^{2}+p y_{f}^{2}\right) / 2 .
$$

Calculating the change of the coordinates per period we find:

$$
\begin{aligned}
& \left(p x_{f}-p x_{i}\right) / z=-\left(\partial F_{00} / \partial q x_{i}\right) / z \\
& \left(q x_{f}-q x_{i}\right) / z=p x_{f}
\end{aligned}
$$

and similarly for the $y$-plane. Defining a function which depends on the initial positions and on the final momenta

$$
<\bar{H}>=F_{00} / z+\left(p x_{f}^{2}+p y_{f}^{2}\right) / 2
$$

we express the result in terms of partial derivatives and $\left(\Delta p x=p x_{f}-p x_{i}, \Delta q x=q x_{f}-q x_{i}\right):$

$$
\begin{aligned}
& \Delta p x / z=-\partial<\tilde{H}>/ \partial q x_{i} \\
& \Delta q x / z=+\partial<\tilde{H}>/ \partial p x_{f}
\end{aligned}
$$

Because $<\tilde{H}>$ does not explicitely depend on $z$, we ignore for a moment the discrete character of $z$. Changing from difference into differential equations for an infinitesimal step length $d z$ of $z$ yields now Hamiltonian's equations:

$$
\begin{aligned}
& d p x / d z=-\partial<H>/ \partial q x \\
& d q x / d z=+\partial<H>/ \partial p x
\end{aligned}
$$

and $<\tilde{H}\rangle$ converges to the averaged Hamiltonian:

$$
\begin{aligned}
<H>= & \left(p x^{2}+p y^{2}\right) / 2+F_{00} / z \\
= & \left(p x^{2}+p y^{2}\right) / 2 \\
& +x_{3}^{2}\left(k_{y}^{2} c x^{2} c y^{2}+k_{x}^{2} s x^{2} s y^{2}\right) /\left(2 k_{y}\right)^{2} .
\end{aligned}
$$

This Hamiltonian agrees with a result presented by [4]. Because of the special choice of our expansion variables, second order terms of this Hamiltonian include already all dominating multipole fields. This shows that the G.F. is a very efficient approach.

An expansion up to 4 th order taken now with respect to $q x$ and $q y$, without constant terms,

$$
\begin{aligned}
<H>\approx & \left(p x^{2}+p y^{2}\right) / 2+\left(x_{3} / 2\right)^{2}\left(\left(k_{y} q y\right)^{2}-\left(k_{x} q x\right)^{2}\right. \\
& \left.+\left(k_{x} q x\right)^{4} / 3-\left(k_{x} k_{z} q x q y\right)^{2}+\left(k_{y} q y\right)^{4} / 3\right)
\end{aligned}
$$

yields the quadrupole and octupole-like terms.

## Numerical Results

A FORTRAN tracking routine is written based on this G.F.. Partial derivatives of the G.F. yields an implicit relation of the particle coordinates at the initial and final point of our transformation. Starting with a set of initial coordinates we apply a Newton fitting routine to solve for the final particle position; a fast and precise technic. Because the transformation is based on a G.F., it becomes fully canonical.

A comparison was done between three different fast tracking methods against a high precision but slow integration routine, splitting the undulator period into more than thousand slices. The calculation was done for a 20 period undulator having a period length of 30 mm , a bending radius of $\rho_{\text {min }}=9.9 \mathrm{~m}$ and a ratio of the $k$-values of $\left(k_{x} / k_{y}\right)^{2}=0.20$.

The fast methods are based on 1) a fast, non-canonical integration routine, splitting the undulator period into 30 steps; fast integration technics like this are applied in the RACETRACK and BETA code; 2) a second order G.F. taking five periods in a single step and 3 ) a third order G.F. taking ten periods in a single step. A set of 16 different, initial coordinates are chosen with values of the order 10 mm and 3 mrad . To get a fair CPU time comparison,
the step length $z$ in each routine is adjusted to achieve roughly equal accuracy of the final coordinates. Results of the different tracking methods at the end of the undulator are shown in the figures. Only discrepancies of the nonlinear part with respect to the high precision routine are shown.

Compared with fast integration routines the reduction in the CPU time was about a factor 50 . However, this reduction depends strongly on the convergence of the expansion. The reduction is still greater when the characteristic bending radius is large as in high energy machines and when the period length becomes short.


Figure caption: For 16 particles with different initial coordinates, the final, non-linear change $\delta$ of the two transversal angle coordinates $x^{\prime}$ and $y^{\prime}$ is compared to the corresponding reference value $\delta_{0}$ of the high precision integration routine: $\Delta=\left(\delta-\delta_{0}\right) / \delta_{0}$.

## References

[1] J. Bahrdt, G. Wüstefeld, A New Tracking Routine for Particles in Undulator and Wiggler Fields; Part I,II and III, BESSY TB Nr. 158 and TB Nr. 163, BESSY GmbH, Berlin, Germany, 1990.
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