Differential Algebra for the Computation of Polarization Dynamics

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The transfer functions of spin and orbit motion can be Taylor expanded with respect to their phase space dependence. An approach for including effects of fringe fields and misalignments on the combined spin–orbit motion in an accelerator is introduced, where care is taken that the orbit map stays symplectic and the spin transfer matrix stays orthogonal in all expansion orders. Concerning fringe fields, this article is a continuation of [1] from purely orbital to coupled spin–orbit motion.

I. INTRODUCTION

The automatic computation of derivatives [2] has been used in accelerator physics since approximately a decade. To illustrate this method, we consider an algorithm mapping a set of numbers $\vec{z}_i$ onto $\vec{z}_f$ represented by $\vec{z}_f = \vec{M}(\vec{z}_i)$. An algorithm which can be evaluated on a computer only requires the evaluation of finitely many elementary operations and elementary functions. Under conditions which are often satisfied, theorems from the field of differential algebras (DA) allow the computation of partial derivatives of such maps $\vec{M}(\vec{z})$ by manipulation of power series [3]. This method of automatically computing all partial derivatives of $\vec{M}$ at some point $\vec{z}_i$ to any previously specified order n is often called DA in the field of accelerator physics. In other words: Given a map $\vec{M}$ which is specified by some algorithm on a computer, then DA allows the automatic computation of the Taylor expansion of $\vec{M}$.

To illustrate how flows of ordinary differential equations (ODEs) can be Taylor expanded, we now consider an ODE $d\vec{z}/dl = \vec{f}(\vec{z}, \vec{\delta}, l)$ which might depend on a set of parameters $\vec{\delta}$. If there is a unique solution for initial conditions $\vec{z}_i$, then $\vec{M}(\vec{z}, \vec{\delta}, l)$ with $\vec{z}(l) = \vec{M}(\vec{z}_i, \vec{\delta}, l)$ is called the flow of the ODE and one can find the solution $\vec{z}(l)$ by propagating the initial condition $\vec{z}_i$ from 0 to l with some numerical ODE solver. We typically use a Runge–Kutta solver of order eight [4]. A program which numerically solves the given ODE for initial values $\vec{z}_i$ is itself an algorithm which evaluates the flow by mapping $\vec{z}_i$ into $\vec{z}(l)$. According to the previous paragraph, evaluating this algorithm with DA leads to a Taylor expansion of the flow $\vec{M}(\vec{z}, \vec{\delta}, l)$ with respect to $\vec{z}$ and $\vec{\delta}$. If the right hand side of the ODE does not depend on the independent variable l, i.e. if $\vec{f}$ only depends on $\vec{z}$ and $\vec{\delta}$, and is

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origin preserving, so that $\vec{f}(0,0) = 0$, then the exponential operator $\vec{M}(\vec{z}, \vec{\delta}, l) = \exp(l\vec{f}^T \vec{\partial}_{\vec{z}})\vec{z}$ can be evaluated in DA [3]. This method of solving an autonomous ODE is faster than numerical integration in DA by up to three orders of magnitude [1,5]. The numerical integration as well as the fast exponential operator technique are implemented in the particle optics code COSY INFINITY [6].

In accelerator physics the motion of particles through a particle optical device is described by a transfer map $\vec{M}(\vec{z}, \vec{\delta}, l)$. Here l describes the arc length along the accelerator, $\vec{z}$ denotes the phase space coordinates of a particle, and $\vec{\delta}$ is a set of parameters of the particle optical device. The map $\vec{M}$ takes initial phase space coordinates $\vec{z}_i$ at arc length 0 into $\vec{z}_f = \vec{M}(\vec{z}_i, \vec{\delta}, l)$ at arc length l. All information concerning the motion of a particle through an accelerator is described by the one turn transfer map. Since the phase space coordinates are usually very small and the parameters of an accelerator do not vary widely, it is often justified to examine the Taylor expansion of the transfer map to some order n with respect to $\vec{z}$ and $\vec{\delta}$. The particles' trajectories are governed by an equation of motion in the form of the ODE mentioned above. DA therefore allows the computation of the nth order Taylor expansion $\vec{M}_n(\vec{z}, \vec{\delta}, l)$, called the Taylor transfer map, of the corresponding flow $\vec{M}(\vec{z}, \vec{\delta}, l)$.

II. SPIN–ORBIT DYNAMICS

The computation of nonlinear Taylor transfer maps of accelerators by the DA method is well established. Computer codes are available that can readily compute the Taylor transfer map $\vec{M}_n(\vec{z}, \vec{\delta}, l)$ of order n corresponding to an equation of motion [6–9]. When the Jacobian $\partial_{\vec{z}}\vec{f}^T$ of the right hand side is a Hamiltonian matrix, then the Jacobian $\partial_{\vec{z}}\vec{M}_n^T$ of the Taylor transfer map is symplectic up to order $n - 1$. For proton storage rings, for the de-

sign of high order spectrographs, and for the correction of aberrations, the symplectic symmetry is very important and should not be violated during computations.

The effort of simulating not only phase space motion but also polarization dynamics has increased lately due to the polarized beam projects at HERA [10] and at RHIC [11] and at lower energy accelerators. Taylor expansions are only justified for small values of the coordinates. When a spin vector of unit length is introduced, a problem occurs since the three spin components are not all small. One could also represent spins by azimuth and polar angle. But again these do not have to be small. Nevertheless, DA techniques can be applied to polarization dynamics [12]. One would like to introduce an approach in which the Taylor expansions are only performed with respect to the optical phase space coordinates $\vec{z}$ not with respect to spin $\vec{s}$.

Such an approach is possible, since the equations of motion contain the spin only linearly

$$\frac{d\vec{s}}{dl} = \vec{\Omega}(\vec{z}, \vec{\delta}, l) \times \vec{s} \implies \vec{s}_f = \underline{A}(\vec{z}_i, \vec{\delta}, l) \cdot \vec{s}_i \qquad (2.1)$$

with the orthogonal spin transfer matrix $\underline{A}(\vec{z}, \vec{\delta}, l)$. This leads to the coupled spin–orbit equation of motion

$$\frac{dz^{(i)}}{dl} = f^{(i)}(\vec{z}, \vec{\delta}, l) \ , \quad \frac{dA_{ij}}{dl} = \epsilon_{ikl}\Omega^{(k)}(\vec{z}, \vec{\delta}, l)A_{lj} \ . \quad (2.2)$$

The Taylor transfer map corresponding to these equations of motion can readily be computed with DA [13]. The Taylor expansion $\underline{A}_n$ to order n of the spin transfer matrix with respect to $\vec{z}$ and $\vec{\delta}$ is orthogonal up to order n since $\underline{A}$ is orthogonal. The orthogonal symmetry preserves the length of the classical spin vector $\vec{s}$ and should therefore not be violated.

III. SYMMETRY PRESERVING APPROXIMATIONS OF FRINGE FIELDS AND MISALIGNMENTS

It was pointed out above that maps of autonomous equations of motion can be found much more efficiently by evaluating an exponential operator than by numerical integration in DA. In figure III the time advantage of the exponential operator method is illustrated for a dipole magnet.
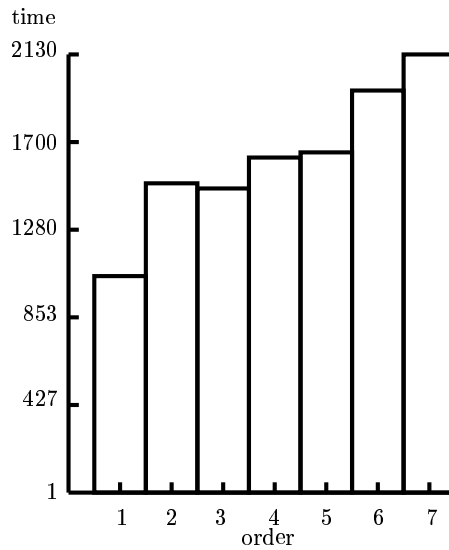

FIG. 1. Time advantage of computing with the exponential operator technique and with numerical integration for obtaining Taylor maps with expansion orders from 1 to 7

Optical elements are often so long that the map is dominated by their main field region, where the field structure does not depend on the arc length l, and the equation of motion becomes autonomous. Nevertheless there are two mayor cases in which the equation of motion becomes non-autonomous. In the so called fringe–field region at the beginning and the end of an element the fields fall off and obviously depend on l. Also, if an element, for example a quadrupole, is tilted and the beam passes through off center, the field structure depends on the arc length. In accelerator physics the computation time required for the DA method would be dominated by computing fringe–field and misalignment effects since solving non-autonomous equations of motion is slower by up to three orders of magnitude.

We therefore searched for efficient approximations of these effects. Due to the importance of the symplectic symmetry of the map $\vec{M}$ and the orthogonal structure of the spin transfer matrix $\underline{A}$, the approximation is not allowed to compromise on these symmetries. For this reason we represent the maps by functions which guarantee the symplectic and orthogonal symmetry even when we approximate these functions. To handle this, we represent the Taylor map $\vec{M}_n$ by its linear part $\vec{M}_1$ and by the polynomial $P_{n+1}(\vec{z}, \delta, l)$ of order $n+1$ which is the Lie exponent of the nonlinear part of the map. To guarantee symplecticity of the linear part of the map, it is represented by a generating function F_i, $i \in \{1, 2, 3, 4\}$ [14, p.382ff],

$$\vec{M}_n(\vec{z}, \vec{\delta}, l) =_n \vec{M}_1 \circ \left(e^{:P_{n+1}(\vec{z},\vec{\delta},l):}\vec{z}\right) \ , \quad F_i \Rightarrow \vec{M}_1 \ . \quad (3.1)$$

The index n on the equivalence sign indicates that the right hand side and the left hand side agree up to order n. The polynomial of order n on the left hand side is therefore computed by evaluating the right hand side up

to order n. If now the second order polynomial F_i and the polynomial of order $n + 1$ in the Lie exponent are approximated in any way, the Taylor map $\vec{M}_n$ computed by equation (3.1) does not describe the phase space motion exactly. However, $\vec{M}_n$ is still exactly symplectic up to order n no matter how crude the approximation is.

The orthogonal spin transfer matrix $\underline{A}$ is represented by $\vec{\gamma}(z, \delta, l) = \sin(\phi/2)\vec{\beta}$ and $\kappa(z, \delta, l) = \cos(\phi/2)$ with the rotation angle ϕ and the rotation axis $\vec{\beta}$ of the rotation matrix $\underline{A}$,

$$A_{ij} = (\kappa^2 - \vec{\gamma}^2)\delta_{ij} + 2\gamma_i\gamma_j - 2\kappa\epsilon_{ijk}\gamma_k . \qquad (3.2)$$

We represent the Taylor expansion $\underline{A}_n$ of the orthogonal matrix by the Taylor expansions κ_n and $\vec{\gamma}_n$ via

$$A_{n,ij} =_n \frac{(\kappa_n^2 - \vec{\gamma}_n^2)\delta_{ij} + 2\gamma_{n,i}\gamma_{n,j} - 2\kappa_n\epsilon_{ijk}\gamma_{n,k}}{\kappa_n^2 + \vec{\gamma}_n^2} . \quad (3.3)$$

$\underline{A}_n$ is now exactly orthogonal up to order n no matter how crudely κ_n and $\vec{\gamma}_n$ are approximated. The denominator is necessary since the approximation might violate $\kappa_n^2 + \gamma_n^2 =_n 1$.

IV. MODES OF APPROXIMATION

The method of symplectic scaling [1,5,15] was implemented to obtain symplectic transfer maps of fringe fields. It is based on the fact that transfer maps in geometrical coordinates as they are used in the code TRANSPORT [16] scale with the geometrical size of the element and with magnetic and electric rigidity.

Geometric scaling relies on a property of the Lorentz force equation for particle coordinates $x(t)$ and momenta $\vec{p}(t)$,

$$\frac{d\vec{p}}{dt} = q(\frac{d\vec{x}}{dt} \times \vec{B} + \vec{E}) . \qquad (4.1)$$

If the magnet's size is scaled by a factor α and the field strength is scaled by a factor $1/\alpha$, then the scaled trajectory $X(t) = \alpha x(t/\alpha)$ and $\vec{P}(t) = \vec{p}(t/\alpha)$ solves the Lorentz equation

$$\frac{d\vec{P}}{dt} = q[\frac{d\vec{X}}{dt} \times \frac{1}{\alpha}\vec{B}(\vec{X}/\alpha) + \frac{1}{\alpha}\vec{E}(\vec{X}/\alpha)] . \qquad (4.2)$$

The T-BMT equation [17,18] of spin motion is also linear in the fields,

$$\frac{d\vec{s}}{dt} = -\frac{q}{m\gamma} \ [\ (1 + G\gamma)\vec{B}_\perp + (1 + G)\vec{B}_\parallel \qquad (4.3)$$

$$+ (\frac{1}{1 + \gamma} + G)\frac{\vec{p} \times \vec{E}}{m} \ ] . \qquad (4.4)$$

Here $G = (g - 2)/2$ is the gyromagnetic anomaly and $\vec{B}_\perp$ and $\vec{B}_\parallel$ are the magnetic field components perpendicular and parallel to $\vec{p}$. Therefore, if $\vec{s}(t)$ describes the spin motion on the trajectory $\vec{x}(t)$, then the spin motion $\vec{S}(t) = \vec{s}(t/\alpha)$ satisfies the T-BMT equation with scaled fields

$$\frac{d\vec{S}}{dt} = -\frac{q}{m\gamma} \ [\ (1 + G\gamma)\frac{1}{\alpha}\vec{B}_\perp(\vec{X}/\alpha) + (1 + G)\frac{1}{\alpha}\vec{B}_\parallel(\vec{X}/\alpha)$$

$$+ (\frac{1}{1 + \gamma} + G)\frac{\vec{p} \times \frac{1}{\alpha}\vec{E}(\vec{X}/\alpha)}{m} \ ] . \qquad (4.5)$$

Geometric scaling can therefore be used simultaneously for phase space and spin motion in coupled electric and magnetic fields.

Rigidity scaling relies on the fact that the Lorentz equation $vd\vec{p}/dl = q\vec{v} \times \vec{B}$, when written with the path length l, leads to the same trajectory through a magnet whenever the magnet rigidity $\frac{qB}{p}$ is not altered. In electric fields $vd\vec{p}/dl = q\vec{E}$ leads to equivalent trajectories as long as $\frac{qE}{vp}$ is not altered. In the T-BMT equation no such scaling exists in a general field arrangement. Including spin motion, one can therefore only use geometric scaling to scale a once computed spin–orbit transport map to an optical element of a different size. It can not be scaled to other field strength or a different energy.

However, when spin–orbit transfer maps for only a small range of energies or field strength are needed, which is for example the case when analyzing spin–orbit motion in the vicinity of a single resonance [19], then we apply a different and much simpler method for approximating a transfer map. We once compute the transfer map at a given energy and a given intermediate field strength B_0 and choose the relative change $\delta_B = (B - B_0)/B_0$ as a parameter of the map. DA then yields a Taylor expansion of the transfer map and also the Taylor expansion of the symplectic and orthogonal representation with respect to this parameter. We store these Taylor expansions of F_i, P_{n+1}, $\vec{\gamma}$, and κ to a file. When the map is later required for a different field strength, we simply insert the appropriate δ_B to obtain an symplectic and orthogonal approximation by the previously described method.

Misalignments are usually small and we therefore similarly approximate the dependence of F_i, P_{n+1}, $\vec{\gamma}$, and κ on the misalignments by Taylor expansions which we compute with DA. These Taylor expansions are stored to a file and are used to approximate the transfer map for any specific misalignment needed. In our applications [19] the Taylor maps of spin–orbit motion have been computed with COSY INFINITY which is written in the foxy language [4]. The symplectic and orthogonal approximations have also been programmed in the foxy language.

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