Advanced computational methods for nonlinear spin dynamics

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Abstract. We survey methods for the accurate computation of the dynamics of spin in general nonlinear accelerator lattices. Specifically, we show how it is possible to compute high-order nonlinear spin transfer maps in SO(3) or SU(2) representations in parallel with the corresponding orbit transfer maps. Specifically, using suitable invariant subspaces of the coupled spin-orbit dynamics, it is possible to develop a differential algebraic flow operator in a similar way as in the symplectic case of the orbit dynamics.

The resulting high-order maps can be utilized for a variety of applications, including long-term spin-orbit tracking under preservation of the symplectic-orthonormal structure and the associated determination of depolarization rates. Using normal form methods, it is also possible to determine spin-orbit invariants of the motion, in particular the nonlinear invariant axis as well as the associated spin-orbit tune shifts.

The methods are implemented in the code COSY INFINITY [1] and available for spin-orbit computations for general accelerator lattices, including conventional particle optical elements including their fringe fields, as well as user specified field arrangements.

1. The One Turn Map for Spin-Orbit Motion

When analyzing the long-term behavior of the dynamics in a storage ring, it is sufficient to consider its behavior on a so-called Poincare plane by a map that describes the transport of beam quantities from the Poincare plane back to itself.

In the conventional model of spin-orbit motion, the orbit dynamics is computed based on the conventional equations of motion[2], and the spin motion is governed by the so-called BMT equation[3] which determines the propagation of the spin vector based on the fields at the current orbit position. The equations of spin-orbit motion are linear in the spin, and hence the transformation of the spin variables can be described in terms of a matrix, the elements of which depend on the orbital quantities only. The orbital quantities themselves are unaffected by the spin motion, such that altogether the map has the form

$$\begin{aligned}\vec{x}_f &= \mathcal{M}(\vec{x}_i)\\ \vec{s}_f &= A(\vec{x}_i)\cdot\vec{s}_i\end{aligned}$$

where $A(\vec{x}) \in SO(3)$ i.e. it is an orthonormal matrix with matrix elements that depend on position. The following study will focus on methods of computing the spin-orbit map and on analyzing it for various quantities that are relevant for the study of the long term behavior of spin motion.

The practical computation of the spin-orbit map can be achieved in a variety of ways. Conceptually the simplest way is to interpret it as a motion in the nine variables consisting of orbit and spin. In this case, the DA method allows the computation of the spin-orbit map in the two conventional ways, namely via a propagation operator for the case of the z-independent fields like main fields, and via integration of the equations of motion with DA [4, 2]. But in this simplest method, the number of independent variables increases from six to nine, which particularly in higher orders entails a rather substantial increase of computational and storage requirements. This limits the ability to perform analysis and computation of spin motion to high orders.

2. Efficient Computation of the Spin-Orbit Map

Due to the special structure of the equations of motion, it is possible to rephrase the dynamics such that it is still described in terms of only the six orbital variables. For this purpose, we derive the equation of motion for the individual elements of the matrix $A(\vec{x})$. To this end, we write $\vec{s}_f = A(\vec{x}) \cdot \vec{s}_i$ and insert this into the spin equation of motion [3]. Comparing coefficients of $\vec{s}$, which only appears linearly, we find that the matrix $A(\vec{x})$ obeys the differential equation

$$A'(\vec{x}) = W(\vec{x}) \cdot A(\vec{x}), \tag{1}$$

where the matrix $W(\vec{x})$ is made from the vector $\vec{w}(\vec{x}) = (w_1, w_2, w_3)$ appearing in the particle optical BMT equation via

$$W(\vec{x}) = \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix}. \tag{2}$$

Integrating the equations of motion for the matrix $A(\vec{x})$ along with the orbital equations now allows the computation of the spin motion based on only six initial variables. Since orthogonal matrices have orthogonal columns, and furthermore their determinant is unity and hence the orientation of a dreibein, is preserved, it follows that the third column of the matrix $A(\vec{x}) = (A_1(\vec{x}), A_2(\vec{x}), A_3(\vec{x}))$ can be uniquely calculated via

$$A_3(\vec{x}) = A_1(\vec{x}) \times A_2(\vec{x}). \tag{3}$$

Thus altogether, only six additional differential equations without new independent variables are needed for the description of the dynamics. For the case of integrative solution of the equations of motion, which is necessary in the case of s-dependent elements, these equations can just be integrated in DA with any numerical integrator.

However, for the case of main fields, the explicit avoidance of the spin variables in the above way is not possible, because for reasons of computational expense, it is desirable to phrase the problem in terms of a propagator operator

$$\begin{pmatrix} \vec{x}_f \\ \vec{S}_f \end{pmatrix} = \exp(\Delta s \cdot L_{\vec{F}}) \begin{pmatrix} \vec{x} \\ \vec{S} \end{pmatrix}. \tag{4}$$

Here $L_{\vec{F}} = \vec{F} \cdot \vec{\nabla}$ is the nine dimensional vector field belonging to the spin-orbit motion. In this case, the differential vector field $L_{\vec{F}}$ describes the whole motion including that of the spin, i.e. $d/ds(\vec{x}, \vec{S}) = \vec{F}(\vec{x}, \vec{S}) = (\vec{f}(x), \vec{w} \times \vec{S})$. In particular, the operator $L_{\vec{F}}$ contains differentiation with respect to the spin variables, which requires their presence. Therefore, the original propagator is not directly applicable for the case in which the spin variables are dropped, and has to be rephrased for the new choice of variables. For this purpose, we define two spaces of functions $g(\vec{x}, \vec{s})$ on spin-orbit phase space as follows:

$$\begin{aligned} X &: \text{ Space of functions depending only on } \vec{x} \\ S &: \text{ Space of linear forms in } \vec{s} \text{ with coefficients in } X \end{aligned}$$

Then we have for $g \in Z$:

$$L_{\vec{F}}\ g = (\vec{f}^t \cdot \vec{\nabla}_{\vec{x}} + (\hat{W} \cdot \vec{s})^t \cdot \vec{\nabla}_{\vec{s}})\ g = \vec{f}^t \cdot \vec{\nabla}_{\vec{x}}\ g = L_{\vec{f}}\ g, \tag{5}$$

and in particular, the action of $L_{\vec{F}}$ can be computed without using the spin variables; furthermore, since $\vec{f}$ depends only on $\vec{x}$, we have $L_{\vec{F}}\ g \in Z$. Similarly, we have for $g = |\ a_1, a_2, a_3 >= \sum_j^3 a_j \cdot s_j \in S$:

$$\begin{aligned} L_{\vec{F}} \mid a_1, a_2, a_3 \ > \ &= (\vec{f}^t \cdot \vec{\nabla}_{\vec{z}} + (\hat{W} \cdot \vec{s})^t \cdot \vec{\nabla}_{\vec{s}})\ (\sum_j^3 a_j \cdot s_j) \\ &= \sum_j (\vec{f}^t \cdot \vec{\nabla}_{\vec{z}}) a_j \cdot s_j + \sum_{j,k} s_j W_{kj} a_k \\ &= \mid L_{\vec{f}} a_1 + \sum_k W_{k1} a_k, L_{\vec{f}}\ a_2 + \sum_k W_{k2} a_k,\ L_{\vec{f}},\ a_3 + \sum_k W_{k3} a_k >, \end{aligned} \tag{6}$$

and in particular, the action of $L_{\vec{F}}$ can be computed without using the spin variables; furthermore, $L_{\vec{F}} \mid a_1, a_2, a_3 > \in S$. Thus, X and S are invariant subspaces of the operator $L_{\vec{F}}$. Furthermore, the action of nine dimensional differential operator $L_{\vec{F}}$ on S is uniquely described by (6), expressing it in terms of the six dimensional differential operator $L_{\vec{f}}$. This now allows the computation of the action of the original propagator $\exp(\Delta s L_{\vec{F}})$ on the identity in R^9, the result of which actually describes the total nine dimensional map. For the upper six lines of the identity, note that the components are in Z, and hence the repeated application of $L_{\vec{F}}$ will stay in Z; for the lower three lines, of the identity map are in S, and hence the repeated application of $L_{\vec{F}}$ will stay in S, allowing the utilization of the invariant subspaces. Since elements in either space are characterized by just six dimensional functions, $\exp(sL_{\vec{F}})$ can be computed in a merely six dimensional differential algebra.

To conclude we note that one turn maps are often made up of small pieces of maps, and it is often necessary to compute the map describing the combination of maps. Let $(\vec{M}_{1,2}, \hat{A}_{1,2})$ and $(\vec{M}_{2,3}, \hat{A}_{2,3})$ be given; then we get

$$\begin{aligned} \vec{M}_{1,3} &= \vec{M}_{2,3} \circ \vec{M}_{1,2} \\ \hat{A}_{1,3}(\vec{z}) &= \hat{A}_{2,3}(\vec{M}_{1,2}) \cdot \hat{A}_{1,2}(\vec{z}); \end{aligned} \tag{7}$$

note the necessity of inserting $\vec{M}_{1,2}$ into $\hat{A}_{2,3}$ before composition.

3. Symplectic Tracking of Spin Motion

Given a spin orbit map $(\vec{M}, \hat{A})$, one of the most immediate applications is the use for tracking of spin dynamics. To this end, the current orbit vector $\vec{z}$ is inserted in $\vec{M}$ and $\hat{A}$, and then the resulting spin matrix is multiplies with the current spin vector$\vec{s}$ to obtain the new spin vector. This method is conceptually straightforward and also very fast, and allows the study of many effects of relevance, in particular long-term depolarization rates.

However, in this particular form, the method has some severe limitations in that it does not preserve the inherent symmetries of the spin-orbit map; specifically, it is known that

(i) The spin map $\hat{A}(\vec{z})$ is orthonormal for any argument $\vec{z}$

(ii) The orbit map $\vec{M}$ is symplectic

However, in the high-order representation of the transfer map, these conditions are only satisfied to the precision with which the expansion of the map represents the true map. While this precision may be high for a single turn, there is the distinct possibilities that the remaining inaccuracies systematically build up over time and limit the long-term accuracy. Thus it is desirable to explicitly restore the two symmetries in each step.

The restoration of the orthonormal symmetry is quite straightforward, since its only detectable consequence is that the spin vector retains its length. The truncation of the spin matrix will entail small violations of this, but these are easily restored by a simple renormalization of the length of $\vec{s}$.

However, the enforcement of the symplectic symmetry is much more complicated because there are many different ways in which motion can be symplectified, and it is desirable to do so with the least overall effect on the predicted orbit motion. Particularly promising are methods that are guaranteed to affect the orbit motion in the smallest possible way, i.e. to afford what is called minimal symplectic tracking. This paper is not the place to delve into details of the underlying complexities, but rather we refer the interested reader to the relevant papers [5, 6, 7, 8, 9].

In order to give an impression of the effects of symplectification as well as the effects of utilizing different orders on the behavior of long term tracking, in figure 1 we show horizontal and vertical tracking in a repetitive system based on transfer maps of order three (top) and 11 (middle). The higher accuracy of the latter case entails a significantly different long-term behavior, with a dynamic aperture that nearly doubles in the horizontal plane and increases by a factor of nearly four in the vertical plane. However, in both horizontal and vertical motion of order 11, there are outer band structures that are not very well defined, and that are actually due to errors in symplectification. The bottom pictures again show tracking to order 11, but now with symplectification based on the EXPO scheme [6, 8]. It is clear that the apparent dynamic aperture increases further, and in addition the outermost structures become more clearly defined and exhibit detailed island structures.

4. Invariant Functions and the Stable Direction of Polarization

However, in addition to merely using the spin-orbit map for efficient tracking, many other important quantities can be obtained directly from the one-turn map. The methods derived here rest on the construction of high order invariant functions, in much a similar way as in conventional normal for methods for orbit motion [10, 2]. Specifically, we call a function $V(\vec{x}, \vec{s})$ an invariant function of the motion if

$$V(\vec{x}, \vec{s}) = V(\mathcal{M}(\vec{x}), A(\vec{x}) \cdot \vec{s}).$$

Considering that in the motion the orbital part is independent of the spin motion as well as the fact that the motion is linear in the spin variables, it is sufficient to consider only functions of the special form

$$V(\vec{x}, \vec{s}) = b(\vec{x}) + \vec{g}(\vec{x}) \cdot \vec{s}.$$

In fact, substituting the expression in the condition of invariance, it follows that b is the usual normal form invariant function of the orbital part of the map, and the search can be restricted to

$$V(\vec{x}, \vec{s}) = \vec{g}(\vec{x}) \cdot \vec{s}.$$

Inserting this into the transfer map, we obtain the necessary condition

$$A(\vec{x}) \cdot \vec{g}(\vec{x}) = \vec{g}(\mathcal{M}(\vec{x})).$$

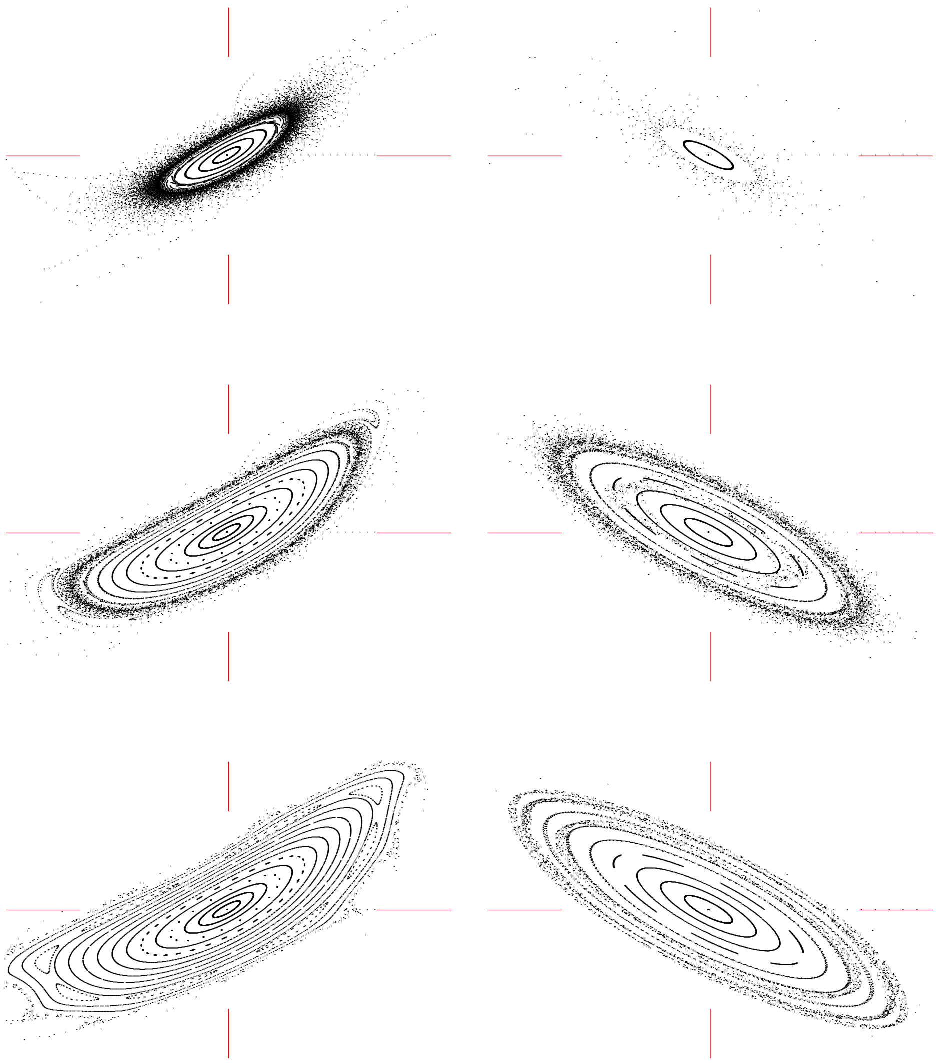

Figure 1. Horizontal and vertical tracking in a repetitive system to orders 3 (top) and 11 (middle) and to order 11 with symplectification (bottom)

In the case $\vec{g}(\vec{0}) \neq 0$, we may even scale the function in such a way that $|\vec{g}(\vec{x}) = 1|$. If the matrix A is not the identity, then this$\vec{g}$ is even unique up to multiplication with invariant functions of the orbital map. The quantity $\vec{g}$ has a rather straightforward interpretation, as it means that the projection of the spin vector on $\vec{g}$ is conserved, and thus it defines an axis along the polarization is conserved.

It has been recognized duly that the existence of an invariant function is highly important, as in practice it allows the injection of a polarized beam along $\vec{g}$ and its preservation for long times. A particular advantage of this definition of $\vec{g}$, which was probably first introduced in[11], is that it does not depend on the Hamiltonian form or the coordinate system or any other specifics of the orbit motion as in the original paper of Derbenev and Kondratenko [12].

5. The Normal Form Algorithm for the Spin-Orbit Map

in this section we provide details about the normal form algorithm for the combined spin-orbit map that allows the computation of spin invariants and in particular the vector$\vec{g}$. Specifically we introduce new variables $\vec{y}$ and $\vec{\xi}$ via

$$\vec{y} = \mathcal{K}(\vec{x}), \vec{\xi} = C\left(\vec{x}\right) \cdot \vec{s},$$

where $C\left(\vec{x}\right) \in SO(3)$. In these variables, the map has the form

$$\begin{aligned} \vec{y}_f &= \mathcal{K}(\mathcal{M}(\mathcal{K}^{-1}(\vec{y}_i))) = \mathcal{N}(\vec{y}_i) \\ \vec{\xi}_f &= C(\mathcal{M}(\mathcal{K}^{-1}(\vec{y}_i))) \cdot A(\mathcal{K}^{-1}(\vec{y}_i)) \cdot C^{-1}(\mathcal{K}^{-1}(\vec{y}_i)) \cdot \vec{\xi}_i = A(\vec{y}_i) \cdot \vec{\xi}_i \end{aligned}$$

The goal is now to show that if there are no resonances up to order m, then the coordinate transformation may be chosen in such a way that the matrix A will up to order n have the form of a simple rotation

$$A(\vec{x}) = \begin{pmatrix} \cos(\lambda(\vec{x})) & \sin(\lambda(\vec{x})) & 0 \\ -\sin(\lambda(\vec{x})) & \cos(\lambda(\vec{x})) & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and in the new variables, the invariant function is simply $V = \xi_3$. The procedure to obtain this form consists of two steps, first a normal form transformation for the orbit part, and then a subsequent transformation for the spin part.

6. The DA Normal Form Algorithm for the Orbital Map

The first process of successive coordinate substitutions to obtain the invariant functions requires to perform the transformation of the orbital map[2]. The starting step consists of the fixed-point transformation and the linear diagonalization. All further steps are purely nonlinear and no longer affect the linear part.

We begin the mth step by splitting the momentary map $\mathcal{M}$ into its linear and nonlinear parts $\mathcal{R}$ and $\mathcal{S}_m$. Then we perform a transformation using a map $\mathcal{K}_m = \mathcal{I} + \mathcal{T}_m$, where $\mathcal{T}_m$ vanishes to order $m-1$. To study the effect of the transformation, we now infer up to order m :

$$\mathcal{K} \circ \mathcal{M} \circ \mathcal{K}^{-1} =_m \mathcal{R} + \mathcal{S}_m + (\mathcal{T}_m \circ \mathcal{R} - \mathcal{R} \circ \mathcal{T}_m).$$

A close inspection of the equation reveals that $\mathcal{S}_m$ can be simplified by choosing the commutator $\{\mathcal{T}_m, \mathcal{R}\} = \mathcal{T}_m \circ \mathcal{R} - \mathcal{R} \circ \mathcal{T}_m$ appropriately; for the full details we refer to [10, 13, 2].

7. The SU(2) Representation of the Spin Map

To reduce the calculations we note that while the orthogonal 3 x 3 matrix $A(\vec{x}) \in SO(3)$ defining the spin part of the map consists of 9 elements, it can be described completely using a smaller number of parameters. We will realize it using the connection between the $SO(3)$ and $SU(2)$ groups. Any matrix $U \in SU(2)$ has the form

$$U = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \text{ where } a \cdot a^* + b \cdot b^* = 1.$$

Corresponding to the vector $\vec{s}$, we define a matrix

$$L = \begin{pmatrix} s_3 & s_1 + is_3 \\ s_1 - is_2 & -s_3 \end{pmatrix}$$

and represent the map in the form

$$\begin{aligned}\vec{x}_f &= \mathcal{M}(\vec{x}_i)\\ L_f &= U(\vec{x}_i)\cdot L_i \cdot U^*(\vec{x}_i)\end{aligned}$$

where $U(\vec{x}) \in SU(2)$ is given as above. Simple arithmetic reveals the following connection between the matrices A and U via

$$A = \begin{pmatrix} \mathrm{Re}(a^2-b^2) & -\mathrm{Im}(a^2+b^2) & -2\mathrm{Re}(ab) \\ \mathrm{Im}(a^2-b^2) & \mathrm{Re}(a^2+b^2) & -2\mathrm{Im}(ab) \\ 2\mathrm{Re}(ab^*) & 2\mathrm{Im}(ab^*) & aa^*-bb^* \end{pmatrix}$$

8. The Normal Form Algorithm for the SU(2) Spin Map

We begin from the spin-orbit map in the form

$$\begin{aligned}\vec{x}_f &= \mathcal{M}(\vec{x}_i)\\ L_f &= U(\vec{x}_i)\cdot L_i \cdot U^*(\vec{x}_i),\end{aligned}$$

where $\mathcal{N}(\vec{x})$ is the normal form of the orbital part of the map up to order m. Consider the coordinate transformation from the old matrix L to the new matrix $\bar{L}$ by the equation

$$L = C(\vec{x})\cdot \bar{L}\cdot C^*(\vec{x}),\ \text{where } C(\vec{x}) \in SU(2).$$

In the new variables, the map has the form

$$\begin{aligned}\vec{x}_f &= \mathcal{N}(\vec{x}_i)\\ \bar{L}_f &= \bar{U}(\vec{x}_i)\cdot \bar{L}_i \cdot \bar{U}^*(\vec{x}_i),\end{aligned}$$

where $\bar{U}(\vec{x}) = C^*(\mathcal{N}(\vec{x}))\cdot U(\vec{x})\cdot C(\vec{x})$. If there are no resonances between orbital and spin tunes up to order m, we can find a matrix $C(\vec{x})$ such that the matrix $\bar{U}(\vec{x})$ will be diagonal up to order m and will have the form

$$\bar{U}(\vec{x}) =_m \mathrm{diag}(\exp(i\kappa(I)), \exp(-i\kappa(I)),$$

where I are the invariants of orbital motion. In this case,

$$A(\vec{x}) =_m \begin{pmatrix} \cos(\lambda(\vec{x})) & \sin(\lambda(\vec{x})) & 0 \\ -\sin(\lambda(\vec{x})) & \cos(\lambda(\vec{x})) & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and the approximate invariant function and spin tune are

$$V = s_3, \lambda(I) = 2\kappa(I).$$

Thus altogether, the normal form algorithms have enabled the direct computation of various quantities of interest in the analysis of spin dynamics in unified way that is applicable to any order desired.

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