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LIE ALGEBRAIC METHODS FOR PARTICLE TRACKING CALCULATIONS*

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I. Introduction

A study of the nonlinear stability of an accelerator or storage ring lattice typically includes particle tracking simulations. Such simulations trace rays through linear and nonlinear lattice elements by numerically evaluating linear matrix or impulsive nonlinear transformations. For large lattices with many nonlinear elements, this can be inefficient because of the necessity of evaluating a separate transformation for each group of linear elements and every individual nonlinear element. Moreover, the validity of the impulsive approximation for nonlinear elements can be questioned. Also, "linear" elements are really not linear. Finally, one must exercise caution to ensure that the transformations employed are exactly canonical.

Using the mathematical tools of Lie groups and algebras, one may construct a formalism which makes explicit use of Hamilton's equations and which allows the description of groups of linear and nonlinear lattice elements by a single transformation. Such a transformation will be exactly canonical and will describe finite length linear and nonlinear elements through third (octupole) order. It is presently possible to include effects such as fringing fields and potentially possible to extend the formalism to include nonlinearities of higher order, multipole errors, and magnet misalignments.

We outline this Lie algebraic formalism and its use in particle tracking calculations. A computer code, MARYLIE, has been constructed on the basis of this formalism. We describe the use of this program for tracking and provide examples of its application.

II. Lie Algebraic Terminology

The behavior of a particle in an accelerator lattice is described by the transfer function of that lattice. This function relates the values of the coordinates and momenta \( \xi = (x, p_x, y, p_y, t, p_t) \) of a particle at some reference location in the lattice to their values \( \xi' = (x', p_x', y', p_y', t', p_t') \) at any other location. We write the dependence of \( \xi' \) on \( \xi \) as follows:

\[
\begin{align*}
\xi' = \tilde{\xi}(\xi)
\end{align*}
\]

(1)

and note that this function may be obtained by solving Hamilton's equations using the particle distance from the reference point, along the design orbit, as the independent parameter. The 6-tuple \( \xi \) is then taken as the initial condition for the calculation. The variables \( x \) and \( y \) are the usual transverse coordinates; \( t \) is the arrival time deviation from the synchronous particle arrival time, and \( -p_t \) is the energy deviation.

The transfer function (1) is a canonical transformation. As such, it admits several representations. A common method of representation is that of expanding (1) in a Taylor series in \( \xi \) and reading off the coefficients of monomials in the expansion. These are the familiar matrix elements of matrix calculations. Alternatively, one may use the language of Lie algebras to represent (1) in a computationally useful fashion.

Let \( f \) and \( g \) be two functions of \( \xi \). The Poisson bracket (PB) is a function of \( \xi \) defined by the following collection of derivatives:

\[
[f, g] = \frac{af}{ax} \frac{af}{ap_x} + \frac{af}{ay} \frac{af}{ap_y} - \frac{af}{at} \frac{af}{ap_t}
\]

(2)

We view the PB as a product of the functions \( f \) and \( g \). Under this product, this set of functions forms a Lie algebra.

Any function \( f = f(\xi) \) generates a Lie operator, denoted by \( \mathcal{f} \), which acts on functions of \( \xi \). This operator, acting on an arbitrary function \( g \), is defined by the rule

\[
\mathcal{f} : g \equiv [f, g] = \mathcal{f} g - g \mathcal{f}
\]

Powers of Lie operators are defined by iterated PB's:

\[
\mathcal{f}^n g = [f, g]_n = [f, [f, g]]_n = [f, [f, [f, g]]]_n = \cdots
\]

and so on.

We may construct sums of Lie operators. In particular, we may define the Lie transformation generated by \( f \) as the following infinite series:

\[
e^{\mathcal{f}} \xi = \sum_{n=0}^{\infty} \frac{\mathcal{f}^n}{n!} \xi = e^{\mathcal{f}} \xi + \frac{1}{2!} [f, [f, \xi]] + \frac{1}{3!} [f, [f, [f, \xi]]] + \cdots
\]

Lie transformations may be used to define canonical transformations. For any \( f = f(\xi) \), the following transformation, defined using a Lie transformation, is canonical:

\[
\tilde{\xi} = e^{\mathcal{f}} \xi = \xi + [f, \xi] + \frac{1}{2} [f, [f, \xi]] + \cdots
\]

Conversely, the factorization theorem tells us that, under quite general conditions, a canonical transformation such as (1) may be written as a product of Lie transformations. Specifically, there exist homogeneous polynomials \( f_2, f_3, f_4, \ldots \) of degree 2, 3, 4, ... in the components of \( \xi \) such that the following transformation reproduces Eq. (1):

\[
\tilde{\xi} = (e^{f_2} e^{f_3} e^{f_4} \cdots) \xi
\]

Moreover, if the infinite product in (2) is truncated at the \( n \)th term, the resulting transformation remains canonical, and will reproduce all terms.
Given the Hamiltonian for the motion of a particle in a particular beamline element, it is possible to compute the polynomials $f_n$ explicitly. One may therefore represent single-element transformations accurately through nonlinearities of high order. This has been done, for a variety of elements, for nonlinearities of third order ($f_3$ is known). It is possible to combine these single-element transformations through use of the Campbell-Baker-Hausdorff theorem. This theorem describes when and how it is possible to combine two Lie transformations to produce a single Lie transformation. The product of two Lie transformations is thereby defined. Using this theorem, we may combine multiple transformations for single elements to produce a single, completely canonical, nonlinear transformation describing the transfer function through a collection of elements.

Lie algebraic methods therefore allow the construction of a canonical transformation which represents the transfer function of an entire lattice accurately through nonlinearities of third order. It is then possible to numerically evaluate this transformation in a completely canonical fashion. This allows tracking of single particle coordinates (ray-traces) for repeated passes through a lattice.

III. Applications to Tracking

The Lie algebraic formalism outlined above has been implemented in the FORTRAN language program MARYLIE (the Maryland Lie Algebraic Transport and Tracking program). MARYLIE represents the exact transfer function for single elements using a third order, completely canonical, approximation of the following form:

$$\xi = e^{f_2} e^{f_3} e^{f_4} \cdots e^{f_n} \xi \text{ = order } n.$$  

The program can combine such transformations for a collection of individual elements to provide a single transformation for the collected elements. This “collective” transformation is also of the form (3) and therefore faithfully represents all effects through those of third (octupole) order in components of $\xi$. Finally, given numerical values for an initial ray $\xi$, MARYLIE can evaluate (3) to obtain numerical values for $\xi$ in a manner which is canonical to all orders. The ray traces are, therefore, completely symplectic.

MARYLIE thus contains remedies for certain deficiencies which can be present in other tracking programs. First of all, it is completely canonical. No spurious damping or growth of emittance (phase space) will occur. Secondly, it incorporates the nonlinear aspects of the so-called linear elements (drifts, dipoles, and quadrupoles). Thirdly, it uses finite length nonlinear elements. This is an advantage in circumstances where impulsive approximations are questionable. Finally, a single transformation may be employed for groups of linear and nonlinear elements. This avoids the inefficiency inherent in providing each nonlinear element with an individual transformation.

It is at this last point, however, that caution must be exercised. It is widely known from experience with tracking simulations, and with the well-known programs TRANSPORT and TURTLE, that nonlinear lattice elements of a given order “cross-couple” to generate effects of even higher order. The program TRANSPORT does not accurately describe all such effects because it omits all matrix products beyond second order. TURTLE, since it tracks elements-to-element, does (numerically) retain these effects.

MARYLIE presently truncates products of Lie transformations to the form (3). Hence, cross-couplings of fourth and higher order are eliminated. The number of elements which can be described by a single transformation is therefore limited. Criteria to quantitatively specify this limit have not yet been developed. Experience with tracking simulations for different types of storage rings indicates, however, that low emittance, very strongly focussing rings (with strong linearities) require more care in this respect than do large emittance rings with weaker focussing and nonlinearities.

Two contrasting examples are given below. In the case of gently focussing high energy lattices, such as one proposed for the SSC, it should be possible to track for many superperiods using a single transformation.

IV. Examples

A. Lawrence Berkeley Laboratory Advanced Light Source

This proposed electron storage ring is to serve as a dedicated synchrotron radiation source for the National Center for Advanced Materials. The 12 cells comprising the lattice consist of strongly focussing pairs of quadrupole triplets. Ring parameters are as follows:

- Circumference: 182.4 m
- Electron energy: 0.9 to 1.9 GeV
- Nominal tunes (H,V): 13.78, 7.78
- Emittance: 6.8x10^-9 m-rad
- Natural chromaticities: -32.0, -17.5
- Maximum quad. gradients: 22.9 T/m
- No. sextupoles: 48

The high chromaticity, low emittance and large quadrupole gradients are characteristic of strongly focussing rings. With activated sextupoles, only a single superperiod may be tracked using one canonical transformation. Truncation errors are observable if a larger number of elements are described using a single mapping. (Even so, this is an advance over other methods, as each superperiod contains four sextupoles. We therefore describe four nonlinear elements using a single transformation). Figure 1 illustrates the result of a MARYLIE bucket height calculation.

B. Los Alamos LAMPF II

One lattice under consideration for a proposed fast cycling synchrotron at Los Alamos would accelerate protons from the LAMPF linac to 32 GeV. This lattice of 60 cells (each consisting of 4 combined-function bends and 4 sextupoles) has nominal tunes of 10.25 (horizontal) and 11.25 (vertical). This lattice can be successfully tracked using a second order matrix based code, provided the tracking is carried out element to element. If, however, single element maps one combined to compute the second order transfer function for an entire cell, and if this cell transfer function is used in tracking, the result exhibits a spurious growth in the single-particle phase space. Figure 2 illustrates this growth in the vertical phase space during 200 turns of cell-to-cell tracking. This effect is purely an artifact of the tracking procedure. It is due to...
the fact that second order matrix transformations for collections of elements are, in general, only through second order (even though the transformations for individual elements may be exactly canonical).

Figure 3 shows the result of tracking with MARYLIE for 48000 turns. This matches the result of tracking element-to-element using the matrix code, but was performed using a transfer function describing 120 cells. Because MARYLIE is completely symplectic, no spurious growth of the vertical phase space is seen; because it is third order, it is possible to track 2 complete turns per transformation without loss of relevant cross-couplings amongst elements.

We therefore conclude that there are cases for which it is very important to maintain the symplectic condition to higher than second order.

V. References

1. For further details consult:


4. The Los Alamos Proton Storage Ring can be tracked 64 turns at a pass (640 lattice periods) using a single transformation when the sextupoles are not activated, and for several turns at a time when sextupoles are activated. A proposed LAMPF II lattice (Ex. B) allows tracking for 2 turns (120 lattice periods) at a pass with activated sextupoles. By contrast, the proposed Advanced Light Source (Ex. A) cannot be tracked for more than one superperiod per transformation without loss of relevant cross-couplings.

5. A description of a Superconducting Super Collider lattice is given by A. Garren in these proceedings. Preliminary calculations indicate that it may be possible to track this lattice for approximately 100 cells per pass with a single transformation using MARYLIE. Thus, there appear to be circumstances where MARYLIE is considerably faster as well as more accurate than impulsive tracking codes such as PATRICIA.

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