AN OVERVIEW OF LIE METHODS FOR ACCELERATOR PHYSICS*

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Abstract

We sketch how Hamiltonian mechanics can be formulated in Lie algebraic terms (indeed Poisson and Jacobi almost invented Lie algebras without knowing it), and how this formulation can be applied to the description and computation of particle orbits in accelerators in a way that both unifies linear and nonlinear theory and leads to explicit results for realistic machines [1–5].

WHAT IS A LIE ALGEBRA?

In grade school we learned how to add numbers to get other numbers, and how to multiply numbers to get other numbers. Mathematicians call an *algebra* any collection of entities for which addition-like and multiplication-like operations are defined.

The concept of numbers and their addition can be extended to the concept of vectors and vector addition. With vectors in mind, is it possible to define multiplication for vectors in such a way that multiplication of any two vectors again yields a vector? There are various possibilities. We will select one. Suppose, for the moment, we denote such multiplication by the symbol $\circ$. Thus, we denote the product of two vectors u and v by the symbols $u \circ v$.

Consider a multiplication rule that has the two properties

$$v \circ u = -u \circ v, \tag{1}$$

$$u \circ (v \circ w) + v \circ (w \circ u) + w \circ (u \circ v) = 0. \tag{2}$$

A multiplication rule with the two properties (1) and (2) is called a *Lie product* rule, and a vector space equipped with a Lie product rule is called a *Lie algebra*. We remark, for reasons which will become evident, that the condition (2) is called the *Jacobi* condition or identity.

IS THERE A LIE ALGEBRAIC STRUCTURE IN HAMILTONIAN MECHANICS?

Notation

Consider a $2n$-dimensional phase space with position coordinates $q_1 \cdots q_n$ and momentum coordinates $p_1 \cdots p_n$. Also, for convenience, introduce the notation

$$z = (q_1 \cdots q_n; p_1 \cdots p_n). \tag{3}$$

That is, z denotes a collection of $2n$ variables with the first n of them being the q's and the remaining n being the p's.

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The Set of Phase-Space Functions Forms a Vector Space

Next let $f(z,t)$ be any function of z and possibly the time t. Evidently, since phase-space functions can be added together and the result is again a phase-space function, the set of all phase-space functions forms a vector space.

The Poisson Bracket Provides a Lie Product

Is there a way of "multiplying" phase-space functions that will satisfy the Lie product requirements (1) and (2)? There is. The *Poisson bracket*, denoted by the symbols $[f,g]$, of any two phase-space functions f and g is defined by the rule

$$[f,g] = \sum_{k=1}^{n} (\partial f/\partial q_k)(\partial g/\partial p_k) - (\partial f/\partial p_k)(\partial g/\partial q_k). \tag{4}$$

Then, it is obvious from its definition that the Poisson bracket has the property

$$[g,f] = -[f,g]. \tag{5}$$

What is not so obvious, and was observed by *Jacobi*, is that the Poisson bracket also has the property

$$[f,[g,h]] + [g,[h,f]] + [h,[f,g]] = 0. \tag{6}$$

Evidently (5) and (6) are analogs of the properties (1) and (2). Only the symbols for a product have been changed, with $\circ$ replaced by $[,]$. We conclude that the set of all phase-space functions with the Lie multiplication rule (4) constitutes a Lie algebra.

The Fundamental Poisson Brackets

Simple calculation shows that for the phase-space coordinates themselves there are the Poisson bracket results

$$[z_a, z_b] = J_{ab}, \ a,b = 1 \cdots 2n \tag{7}$$

where J is the $2n \times 2n$ matrix, called the Poisson matrix,

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{8}$$

Here 0 and I denote the $n \times n$ zero and identity matrices.

A RELATED LIE ALGEBRA IN HAMILTONIAN MECHANICS

Lie Operators

Given any phase-space function $f(z,t)$ there is a related differential operator, called a *Lie operator* and denoted by the symbols $:f:$, defined by the rule

$$:f: = \sum_{k=1}^{n} (\partial f/\partial q_k)(\partial/\partial p_k) - (\partial f/\partial p_k)(\partial/\partial q_k). \tag{9}$$

Evidently, the action of $: f :$ on any function $g(z,t)$ is given by the relation

$$: f : g = \sum_{k=1}^{n} (\partial f/\partial q_k)(\partial g/\partial p_k) - (\partial f/\partial p_k)(\partial g/\partial q_k) = [f,g]. \quad (10)$$

We may view a Lie operator as a Poisson bracket waiting to happen.

Lie Operators Form a Lie Algebra

Since differential operators can be added and the result is again a differential operator, Lie operators form a vector space. Can the set of Lie operators also be given a Lie product rule? Let $\{: f :, : g :\}$ denote the *commutator* of the Lie operators $: f :$ and $: g :$,

$$\{: f :, : g :\} =: f :: g : - : f :: g : . \quad (11)$$

It is easily verified that the commutator satisfies requirements analogous to the Lie product requirements (1) and (2). Therefore one suspects that Lie operators might also form a Lie algebra with the Lie product symbol $\circ$ replaced by the symbols $\{,\}$. But is the commutator of two Lie operators again a Lie operator? It is. It can be shown from the Jacobi identity (6) that there is the beautiful relation

$$\{: f :, : g :\} =: [f,g] : . \quad (12)$$

Powers of Lie Operators

Based on the definition of a Lie operator, we can also define powers $: f :^{\ell}$ of Lie operators by the rules

$$: f :^{0} g = g, \quad (13)$$

$$: f :^{1} g =: f : g = [f,g], \quad (14)$$

$$: f :^{2} g = [f,[f,g]], \text{ etc.} \quad (15)$$

Lie Transformations

With powers of Lie operators defined, we can also define power series. A particularly important power series, called a *Lie transformation*, is that based on the Taylor coefficients of the exponential function and given by the rule

$$\exp(: f :) = \sum_{\ell=0}^{\infty} : f :^{\ell} /\ell!. \quad (16)$$

When applied to any function g, it follows that there is the result

$$\exp(: f :) g = \sum_{\ell=0}^{\infty} : f :^{\ell} g/\ell! = g + [f,g] + [f,[f,g]]/2! + \cdots . \quad (17)$$

INTEGRATING HAMILTON'S EQUATIONS OF MOTION AND SYMPLECTIC MAPS

Transfer Maps Arising from Hamiltonians

Suppose $H(z,t)$ is some Hamiltonian. Following Hamilton, it produces the set of first-order equations

$$\dot{q}_j = \partial H/\partial p_j, \quad (18)$$

$$\dot{p}_j = -\partial H/\partial q_j, \quad (19)$$

which can be written more compactly in the form

$$\dot{z}_a = - : H : z_a. \quad (20)$$

Let z^{in} denote a set of *initial* conditions at the initial time t^{in}, and suppose the equations of motion (20) are integrated to a *final* time t^{fin} to find final conditions z^{fin}. We may view the relation between z^{fin} and z^{in} as a *map* $\mathcal{M}$, often called a *transfer map*, that sends phase space into itself, and write

$$z^{fin} = \mathcal{M} z^{in}. \quad (21)$$

Effect of Small Changes in the Initial Conditions

Suppose we make small changes dz^{in} in the initial conditions. According to calculus, doing so will produce small changes dz^{fin} given by the relation

$$dz^{fin} = M(z^{in}) dz^{in} \quad (22)$$

where $M(z^{in})$ is the *Jacobian matrix* defined by

$$M(z^{in})_{ab} = \partial z_a^{fin}/\partial z_b^{in}. \quad (23)$$

The Symplectic Condition

If $\mathcal{M}$ arises from integrating Hamilton's equations of motion (20) for some Hamiltonian, as we have assumed, then it can be shown that $M(z^{in})$ must satisfy the (nonlinear) condition

$$M^T(z^{in}) J M(z^{in}) = J \quad (24)$$

for all z^{in} where M^T denotes the transpose of M. Matrices M that satisfy (24) are called *symplectic* matrices, and correspondingly maps $\mathcal{M}$ whose Jacobian matrices $M(z^{in})$ satisfy (24) for all z^{in} are called sympletic maps.

We have learned that integrating Hamilton's equations of motion produces symplectic maps. Conversely, it can be shown that every symplectic map arises from integrating Hamilton's equations of motion for some Hamiltonian. Thus, finding symplectic maps and solving Hamilton's equations of motion are equivalent tasks.

Taylor Representation of Transfer Map

Suppose some design orbit has been found, and now let the quantities z_a be *deviation* variables about the design orbit. In terms of these variables, $\mathcal{M}$ sends the origin into

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itself. Moreover, suppose the Hamiltonian is analytic in z so as to have a convergent Taylor expansion of the form

$$H(z,t) = \sum_{m=2}^{\infty} H_m(z,t) \tag{25}$$

where each $H_m(z,t)$ is a homogeneous polynomial (in the components of z) of degree m. Then the final and initial conditions will be related by Taylor expansions of the form

$$\begin{aligned} z_a^{fin} &= \sum_b R_{ab} z_b^{in} + \sum_{bc} T_{abc} z_b^{in} z_c^{in} \\ &+ \sum_{bcd} U_{abcd} z_b^{in} z_c^{in} z_d^{in} + \cdots . \end{aligned} \tag{26}$$

We note that the Taylor coefficients R_{ab}, T_{abc}, U_{abcd}, etc., occurring in (26) are not all independent, but rather are interrelated by the symplectic condition (24). The matrix R must be symplectic, and the entries in R, T, U, etc. are interrelated in a complicated way.

IS THE LIE ALGEBRAIC STRUCTURE OF HAMILTONIAN MECHANICS OF ANY USE?

Lie Representation of Transfer Map

Suppose $\mathcal{M}$ is a symplectic map that sends the origin into itself. It can be shown that any such map has the factorization

$$\mathcal{M} = \mathcal{R} \exp(: f_3 :) \exp(: f_4 :) \exp(: f_5 :) \cdots \tag{27}$$

where $\mathcal{R}$ is a linear symplectic map whose action is described by the symplectic matrix R and the f_m are homogeneous polynomials of degree m in the phase-space variables z^{in}. Moreover, unlike the Taylor representation (26), the homogeneous polynomials f_m are all independent. Any choice for the f_m produces a symplectic map, and every (origin preserving) symplectic map has a unique factorization of the form (27). Thus, in the case of accelerator physics, the effect of any beam-line element or collection of such elements, including the one-turn map for a circular machine, is characterized by a symplectic matrix R and a collection of polynomials f_m; and the symplectic condition is automatically built into the description. In particular, it can be shown that $\mathcal{R}$ describes linear behavior about the design orbit, f_3 describes second-order (such as might be caused by sextupoles) and yet higher-order effects, f_4 describes third-order (such as might be caused by octupoles) and yet higher-order effects, etc.

We also remark, in passing, that $\mathcal{R}$ can be written in terms of Lie transformations. In general there are two unique quadratic polynomials called f_2^c and f_2^a (where the superscripts c and a characterize the matrices associated with the polynomials as *commuting* or *anti-commuting* with J) such that there is the relation

$$\mathcal{R} = \exp(: f_2^c :) \exp(: f_2^a :). \tag{28}$$

In some important cases a single f_2 suffices, and its coefficients are related to phase advances and *Twiss* parameters.

Finally, in the case that $\mathcal{M}$ does not send the origin into itself, there is a first-degree polynomial f_1 such that $\mathcal{M}$ has the unique factorization

$$\mathcal{M} = \exp(: f_1 :) \mathcal{R} \exp(: f_3 :) \exp(: f_4 :) \cdots . \tag{29}$$

It can be verified that the Lie transformation $\exp(: f_1 :)$ produces translations in phase space, and describes the error effects of beam-line element misplacement or misalignment or (in the case of dipoles) mis-powering.

Lie Formulas for Multiplying/Concatenating Symplectic Maps

Given any two Lie transformations there are Lie algebraic rules for combining them. In particular there is a rule for manipulating exponents, called the *Baker-Campbell-Hausdorff* (BCH) theorem/series, that along with (12) leads to the result

$$\exp(: f :) \exp(: g :) = \exp(: h :) \tag{30}$$

with

$$\begin{aligned} h &= f + g + (1/2)[f,g] \\ &+ (1/12)\{[f,[f,g]] + [g,[g,f]]\} + \cdots . \end{aligned} \tag{31}$$

In the context of accelerator physics, suppose the transfer map for each beam-line element is known in the standard forms (27) or (29). Then the BCH theorem can be used to manipulate the various exponents appearing in the individual maps to again rewrite the product of the maps in standard form. That is, there are procedures for finding the net map for a full beam line, or any portion thereof, given the maps for the individual elements. In the case of case of a circular machine, one can combine all the maps for the individual beam-line elements together to find a full one-turn map, or even a several-turn map. Finally, the BCH theorem also provides a procedure for inverting symplectic maps.

Normal Form for a Symplectic Map

Suppose $\mathcal{M}$ is the one-turn map for a circular machine, and the machine tunes are not resonant. Then there is symplectic map $\mathcal{A}$, called the *transforming* or *normalizing* map, such that the map $\mathcal{N}$ given by

$$\mathcal{N} = \mathcal{A}\mathcal{M}\mathcal{A}^{-1} \tag{32}$$

has a particularly simple form, called a *normal* form. The normal-form process is the nonlinear analog of the concept of matrix diagonalization.

It can shown that $\mathcal{N}$ contains all information about tunes, anharmonicities, and chromaticities to any desired order; and $\mathcal{A}$ contains all information about linear and nonlinear lattice functions. The map $\mathcal{A}$ can also be used to construct nonlinear generalizations of the Courant-Snyder invariants, to analyze tracking data for the presence of KAM tori, and to generate matched beams including nonlinear effects.

Computing Symplectic Maps $\mathcal{M}$

Given a Hamiltonian H, it can be shown that $\mathcal{M}$ obeys the equation of motion

$$\dot{\mathcal{M}} = \mathcal{M} : -H : . \tag{33}$$

Suppose H expanded in the form (25). How does one find the corresponding map $\mathcal{M}$ in the form (27)? We will first describe how R can be found, and then describe how the f_m can be found. Actually, it is computationally simpler to write $\mathcal{M}$ in the *reverse* factorized form

$$\mathcal{M} = \cdots \exp(: g_5 :) \exp(: g_4 :) \exp(: g_3 :) \mathcal{R}, \tag{34}$$

and then find the g_m. Once they are known the f_m can be found from the g_m by using concatenation formulas to bring (34) to the standard forward factorized form (27).

Finding R Since $H_2(z,t)$ is quadratic in the variables z, it can be written in the form

$$H_2(z,t) = (1/2) \sum_{ab} S_{ab}(t) z_a z_b \tag{35}$$

where $S(t)$ is a symmetric matrix. It can be shown that R is the solution to the matrix differential equation

$$\dot{R}(t) = JS(t)R(t) \tag{36}$$

with the initial condition

$$R(t^{in}) = I. \tag{37}$$

If S is time independent, (36) with the initial condition (37) can be integrated immediately to give the result

$$R(t) = \exp[(t - t^{in})JS]. \tag{38}$$

If S is time dependent, as will be the case if one wishes to include fringe-field effects (recall that here t plays the role of s, distance along the design orbit), then (36) must be integrated numerically.

Finding the g_m In general to find the g_m one must first transform the $H_m(z,t)$, with $m \geq 3$, to the *interaction picture* specified by $H_2(z,t)$ in a manner analogous to similar calculations in Quantum Mechanics. Define interaction picture Hamiltonian pieces $H_m^{int}(z,t)$ by the rule

$$H_m^{int}(z,t) = H_m(Rz,t) \text{ with } m \geq 3. \tag{39}$$

Then it can be shown that the g_m with $m \geq 3$ obey equations of motion of the form

$$\dot{g}_3 = -H_3^{int}, \tag{40}$$

$$\dot{g}_4 = -H_4^{int} + (: g_3 : /2)(-H_3^{int}), \text{ etc.} \tag{41}$$

with the initial conditions

$$g_m(z, t^{in}) = 0. \tag{42}$$

Presently explicit differential equations of this kind for the g_m have been worked out through $m = 8$.

In the approximation that $H_m(z,t)$ is t independent within each beam-line element, which amounts among other things to the neglect of fringe-field effects, there are a variety of ways for obtaining the g_m either analytically or numerically. If $H_m(z,t)$ is t dependent, as will be the case if fringe-field effects are to be taken into account, then the equations of the form (40), (41), etc. must be integrated numerically with the initial conditions (42).

Computing $\mathcal{M}$ for Realistic Beam-Line Elements: Use of Surface Methods

In this final subsection we will describe how to compute accurate transfer maps for realistic beam-line elements including all fringe-field and multipole effects. For simplicity we will limit our discussion to magnetic beam-line elements. Analogous treatments can be applied to the cases of electrostatic and RF electromagnetic fields.

In the previous subsection it was assumed that the $H_m(z,t)$ are given, which is equivalent, in the case of accelerator physics and the treatment of magnetic beam-line elements, to the assumption that the vector potential $\boldsymbol{A}$ for the the magnetic field $\boldsymbol{B}$ is known in analytic form so that a Taylor expansion can be performed to find the $H_m(z,t)$. That is, high-order spatial derivatives of $\boldsymbol{A}$ are needed about the design orbit.

However suppose, as is often the case, that only $\boldsymbol{B}$ is known, and moreover it is only known at a 3-D collection of grid points. For example, when iron is present, $\boldsymbol{B}$ can only be found numerically at a collection of grid points with the aid of some three-dimensional electromagnetic solver. What can be done then to find $\boldsymbol{A}$ and its high-order derivatives?

At first thought one might contemplate using numerical differentiation of grid-point data to determine $\boldsymbol{A}$ and its spatial derivatives. But it is well known to numerical analysts that numerical differentiation of grid-point data is intolerably sensitive to numerical noise in the data. Each differentiation operation amplifies noise. And it is high-order derivatives that are needed to compute $\mathcal{M}$ to high order.

This problem can be overcome, at least to reasonably high order, by the use of *surface methods*. By a theorem of *Neumann* the values of $\boldsymbol{B}$, and accordingly the associated values of $\boldsymbol{A}$, can be found within any volume V if the normal component of $\boldsymbol{B}$ is known on any surface S that bounds V. Moreover, it can be shown that the process of determining interior fields from fields on a surrounding surface is *smoothing*. That is, the interior field values are relatively insensitive to noise in the surface data. Finally, it can be shown that this smoothing overcomes the amplification of numerical noise associated with differentiation.

Straight beam-Line Elements There are two cases to be considered: straight (or essentially straight) beam-line elements, and curved beam-line elements with significant

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sagitta. In the case of straight beam-line elements it is possible to surround the design orbit by an imaginary cylinder. This cylinder can be conveniently assumed to have a circular, elliptical, or rectangular cross section. Circular cylinders are natural for the case of quadrupoles, sextuples, octupoles, etc. Cylinders with elliptical or rectangular cross sections may be more appropriate for elements for which the bore width is larger than the gap height. See Figure 1 for the case of a wiggler.

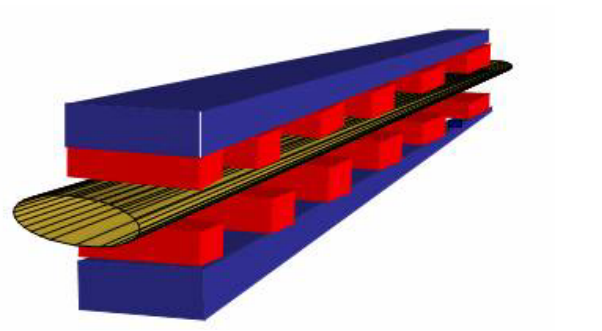

Figure 1: An elliptical cylinder, centered on the z-axis, fitting within the bore of a wiggler, and extending beyond the fringe-field regions at the ends of the wiggler.

For these cylindrical volumes V and their associated surfaces S it is possible to solve *Laplace's* equation by separation of variables. From these solutions it is possible to generate explicit formulas that determine $\boldsymbol{A}$ and its spatial derivatives at any interior point in terms of values of the normal component of $\boldsymbol{B}$ at selected grid points on S, and consequently the $H_m(z,t)$ can be found. The required surface values can be determined by extrapolation of the 3-D grid-point numerical values of $\boldsymbol{B}$ onto the selected grid points on S. Finally, the equations (36), (40), (41), $\cdots$ can be integrated to yield $\mathcal{M}$.

Curved beam-Line elements For curved beam-line elements with significant sagitta it is impossible to fit a straight cylinder within the bore of the element. In this case it is necessary to employ volumes V, and their associated surfaces S, that have a more complicated geometry. Figure 2 shows a convenient surface for the case of dipoles with significant sagitta, the surface of a bent box with straight end legs.

Unfortunately, for curved beam-line elements there are no geometries for which the Laplace equation is separable and therefore, while the results of Neumann still hold, there is no way to exploit them by explicit formulas. However, according to a theorem of *Helmholtz*, interior fields can also be computed from surface data providing *both* the normal component of $\boldsymbol{B}$ and the scalar potential ψ associated with $\boldsymbol{B}$ are known on the surface. Moreover, in this case the interior vector potential and its spatial derivatives can be found by multiplying the surface data by *known geometry-independent* kernels and then integrating the results over S.

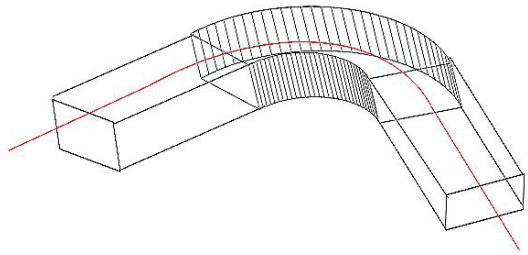

Figure 2: A bent box, fitting within a dipole, and having straight end legs that extend beyond the fringe-field regions at the entry and exit of the dipole.

Finally, this process is also smoothing: the interior values of $\boldsymbol{A}$ and its spatial derivatives so obtained are also relatively insensitive to noise in the surface data.

In practice, the procedure is as follows: First set up cubature points (specially selected grid points) on S, interpolate the numerical 3-D grid data for $\boldsymbol{B}$ onto the surface cubature points, and compute the normal component of $\boldsymbol{B}$ at these cubature points. In addition interpolate 3-D grid data for ψ, which can also be provided by 3-D electromagnetic solvers, onto the surface cubature points. Next multiply the surface data by the known kernels and integrate the results over the surface using cubature formulas. The result will be the interior vector potential and its spatial derivatives, and consequently the $H_m(z,t)$ can be found. Finally, the equations (36), (40), (41), $\cdots$ can be integrated to yield $\mathcal{M}$.

CONCLUSION

For both straight and curved beam-line elements, the use of Lie and surface methods makes it possible to compute, for the first time, accurate high-order transfer maps for realistic elements including all fringe-field and multipole error effects.

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