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LIE ALGEBRAIC TREATMENT OF LINEAR AND NONLINEAR BEAM DYNAMICS

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1. INTRODUCTION

This chapter is written for readers from diverse backgrounds. For readers with little accelerator physics or beam dynamics background, all that is presumed is a passing acquaintance with the fact that charged-particle optical systems are composed of drift spaces, dipole bending magnets, quadrupole focusing magnets, and other beam-line elements, and that in certain circumstances particles in such systems perform betatron oscillations. It is hoped that such readers will be intrigued to learn more about the fascinating field of accelerator physics and charged-particle beam dynamics.

For readers who already have a background in this field, it is hoped that they will enjoy and benefit from seeing the subject from yet another perspective. To such readers we apologize in advance for the fact that although many topics deserve some mention, with limited space the treatment of each selected topic is necessarily brief, and many equally important topics have not been treated at all.

1.1 *New Methods*

The purpose of this paper is to present a summary of new methods, employing Lie algebraic tools, for characterizing beam dynamics in charged-particle optical systems. These methods are applicable to accelerator design, charged-particle beam transport, electron microscopes, and also light optics. The new methods represent the action of each separate element of a compound optical system, including all departures from paraxial optics, by a certain operator. The operators for the various elements can then be concatenated, following well-defined rules, to obtain a resultant operator that characterizes the entire system.

This paper deals mostly with accelerator design and charged-particle beam transport. The application of Lie algebraic methods to light optics and electron microscopes is described elsewhere (1; see also 44). To keep its scope within reasonable bounds, we restrict our treatment of accelerator design and charged-particle beam transport primarily to the use of Lie algebraic methods for the description of particle orbits in terms of transfer maps. There are other Lie algebraic or related approaches to accelerator problems that the reader may find of interest (2). For a general discussion of linear and nonlinear problems in accelerator physics see (3).

The use of Lie algebraic tools has several benefits. First, the calculation of high order nonlinear effects is facilitated. As an example, this paper describes procedures that are currently implemented through third (octupole) order in the computer programs MARYLIE 3.0 and MARYLIE 3.1, and soon will be implemented in the program MARYLIE 5.1 through fifth (12-pole) order. The program MARYLIE 3.0 is described in (4). The foundations of MARYLIE 3.1 and MARYLIE 5.1 are described in (5; see also 26, 28). [The name MARYLIE honors Henrietta Maria, the queen of England after whom the state of Maryland is called, and Sophus Lie, the discoverer of Lie algebras.]

Second, Lie algebraic tools provide an optimal method for characterizing optical systems. Consequently, their use is expected to minimize computer storage, maximize computational speed, and facilitate communication, insight, and improved design.

Finally, Lie algebraic tools and associated group-theoretic concepts both suggest entirely new ways of looking at problems and provide a powerful calculus for analyzing and describing the behavior of optical systems. In particular, it should be possible eventually to analyze and control nonlinear behavior with the same facility and completeness with which we now handle linear behavior.

In order to dispel any possible misconceptions or illusions of grandeur at this point, it should be stated that there is nothing that can be computed

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Old Methods

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1 An optical system
A particle originates
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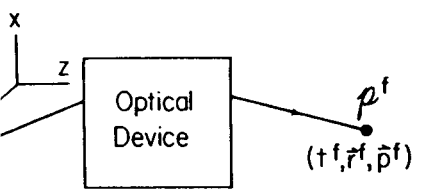
ıods that could not in principle be computed
rbation theory or, indeed, Newton's equations.
ause of their concise and modular nature, the use
has made it possible to obtain many results well
vailable by any other method.

n illustrated schematically in Figure 1. A charged
initial point P^i at time t^i. After moving through
ically containing various electric and magnetic
at the final point P^f at time t^f. What we have
device may be, for example, a single beam-line
rt system, or an entire accelerator. Given the
nd momenta $(t^i, \mathbf{r}^i, \mathbf{p}^i)$, the fundamental problem
is to determine the final quantities $(t^f, \mathbf{r}^f, \mathbf{p}^f)$ and
ce in such a way that the relation between the
has various desired properties.
he initial and final quantities can always in prin-
grating numerically the equations of motion.
v numerical integration has been and is used to
ccuracy of various Lie algebraic maps and ray-
also 31, 33). However, high accuracy numerical
y slow if performed for a large number of rays, or
the long-term behavior of even a few trajectories.
one does not necessarily give great insight into
al system or what could be done to improve it.
be regarded more as proof of the pudding rather
good pudding.
cedures, which may be viewed as high speed (but
integration methods, have been developed for use
e such procedure is to approximate trajectories



nsisting of an optical device preceded and followed by simple
P^i at time t^i with location $\mathbf{r}^i$ and momentum $\mathbf{p}^i$ and terminates
and momentum $\mathbf{p}^f$.

in drifts, dipoles, and quadrupoles by linear transformations, and to approximate trajectories in sextupole, octupole, and higher order multipole fields by simple impulsive kicks. The computer codes PATRICIA, PATRIS, and RACETRACK use this procedure. PATRIS was created by A. Ruggiero at Brookhaven National Laboratory. For the other codes see (7). This procedure has the advantage that it can in principle treat nonlinear (multipole) effects of arbitrarily high order. It has the disadvantage that intrinsic and fringe-field aberration effects in dipoles and quadrupoles are ignored. Also, finite-length effects are lost in multipoles. These latter effects can be recovered by subdividing the multipoles (thereby increasing the number of kicks), but only at the cost of reduced computational speed.

A second such procedure is to treat trajectories in drift spaces exactly, and to approximate trajectories in all other elements by impulsive kicks. This approach has the feature that it becomes exact (arbitrarily accurate), save for fringe-field effects, in the limit that the subdivision of the elements becomes arbitrarily fine. Of course, this improvement in accuracy is again at the expense of reduced computational speed, and at some stage round-off error can also become a problem. The computer code TEAPOT uses this procedure, and is an example of what may be called a symplectic integrator. [A symplectic integrator is a numerical integrator that exactly preserves the symplectic condition (described in Section 2.3 of this paper).] For a further description of symplectic integrators, see (8, 51). For a description of TEAPOT, see (9).

An approach complementary to direct ray tracing is to seek and employ some sort of functional representation for the relation between initial and final quantities. As described in Section 2.2, such an approach uses the concept of transfer maps.

There are currently three procedures for representing transfer maps. One commonly used and very fruitful procedure, often referred to as a higher order matrix method, is to expand the final quantities as a power series in the initial quantities. In lowest order, this procedure yields the linear matrix approximation of paraxial optics. The computer code SYNCH and many other "linear" codes employ the linear matrix approximation. These codes are often supplemented with the ability to trace rays through nonlinear elements in the kick approximation, and with various analytic procedures for computing nonlinear effects. For a description of SYNCH, see (10). For a description of several programs, see (11). The higher order (nonlinear) terms in such an expansion provide a description in terms of aberration coefficients. The number of these aberration coefficients grows very rapidly with order. Also, as discussed below they are not all independent.

The widely used code TRANSPORT originally computed aberration coefficients through second order, and more recently computes through third order. The second-order version of TRANSPORT is described by Brown et al. (12). For a more extensive description of TRANSPORT methods, see Carey (13). The code DIMAD is based on TRANSPORT, and is tailored for the treatment of circular machines (14). The code MAD is a shell (with a particularly powerful input and command structure) that is intended to contain within it the essence of many of the codes listed in the references above. It is described by Iselin & Niederer (15). The code GIOS computes aberration coefficients through third order with an emphasis on spectrometer design (16). The program COSY 5.0 computes aberration coefficients through fifth order (17). The codes FASTRACK and THINTRAC employ both kick (symplectic integration) methods and transfer map (including their Lie algebraic representation) methods (18).

A second procedure is to describe the relation between final quantities and initial quantities by means of various generating or characteristic functions. The method of characteristic functions or eikonals is widely used in light optics (19) and in the design of electron microscopes (20). More recently, the method of characteristic functions has been applied to accelerators (21).

Despite their general theoretical importance and frequent applicability, there are also certain awkward features associated with the use of characteristic functions. For example, their use gives relations that are implicit in that they contain an admixture of initial and final quantities. These relations must be made explicit, by solving for the final quantities in terms of the initial quantities, before they can be applied. This same circumstance makes it difficult to find explicitly the characteristic function for a compound optical system even when the characteristic function for each of its component parts is already known. It may also be observed that, when characteristic functions are used, no one kind of characteristic function is applicable to all kinds of optical systems. For example, a point characteristic function is not applicable to an imaging system, and an angle characteristic function is not applicable to a telescopic system.

The third procedure employs Lie algebraic methods, and is the subject of this paper. It should be stressed at this point that all three procedures produce and carry the same mathematical information. That is, given the results of one of these procedures, it is possible to compute the equivalent results for each of the other two. The computation of Lie algebraic results from aberration coefficients is described in (22, 24, 44, 52). The computation of characteristic functions from Lie algebraic results is described in (36). Also, each procedure has its own utility. Thus, it is useful to be able to exploit all of them. For example, although the various MARYLIE codes use Lie algebraic methods, they can also produce power series (aberration) expansions upon command, and can employ these series for various purposes including fitting and ray tracing. If desired, the MARYLIE codes can also produce a characteristic generating function and employ it for ray tracing.

1.3 *Promises*

As indicated earlier, the purpose of this chapter is to summarize an alternative Lie algebraic approach to the problem of characterizing charged-particle optical systems and charged-particle beam dynamics. This approach exploits the fact that the equations of motion for charged particles in electromagnetic fields can be written in Hamiltonian form. In particular, it is possible to represent the action of each separate element of a compound optical system, including all departures from linear matrix optics, by a certain operator. These operators can then be concatenated by following well-defined rules to obtain a resultant operator that charcterizes the entire system. Finally, this resultant operator can be analyzed using various Lie algebraic and group-theoretic methods in order to determine the performance of the system.

The remaining sections of this review are devoted to an exposition of Lie algebraic methods and examples of their use. Section 2 treats the symplectic condition, its effect on aberration expansions, and its group-theoretic consequences. Section 3 provides a summary of elementary Lie algebraic methods. Advanced Lie algebraic methods are introduced in Section 4. Two final sections describe elementary and advanced applications of these methods.

2. SYMPLECTIC MAPS

2.1 *Coordinates*

Suppose trajectories are described by general coordinates $q_1, \ldots, q_n$ and their conjugate momenta $p_1, \ldots, p_n$. (Here n, the number of degrees of freedom, will usually equal 3, but at this point it is possible to keep the discussion completely general.) The canonical coordinates q, p are not necessarily those used in Section 1.2. Often it is useful to take some coordinate rather than time as the independent variable, and to treat time as a dependent variable (22).

It is convenient to treat both the q and p equally. This can be done by introducing the quantities $z_1, \ldots, z_{2n}$ by the prescription

$$z = (q, p). \qquad 1.$$

That is, the first n components of z ($z_a, a = 1, 2, \ldots, n$) are the quantities

$q_1, \ldots, q_n$, and the last n components of z ($z_a, a = n+1, \ldots, 2n$) are the quantities $p_1, \ldots, p_n$.

2.2 *Aberration Expansions*

Employing a notation analogous to that used in Figure 1, suppose an incoming initial trajectory is specified by the phase-space coordinates z^i, and that the outgoing final trajectory has the corresponding phase-space coordinates z^f. Now invoke the spirit of Brook Taylor to expand the components of z_f as a power series in the components of z^i. Such an expansion produces a general expression of the form

$$z_a^f = K_a + \sum_b R_{ab} z_b^i + \sum_{bc} T_{abc} z_b^i z_c^i + \sum_{bcd} U_{abcd} z_b^i z_c^i z_d^i + \cdots. \qquad 2.$$

The matrix R is called the (first-order) transfer matrix, and the quantities T, U, etc are called higher order transfer matrices, or alternatively, aberration coefficients.

Equation 2 describes a relation between z^i and z^f that we will view as a mapping $\mathcal{M}$ of z^i into z^f. Thus, it is convenient to write Equation 2 in the more compact form

$$z^f = \mathcal{M} z^i. \qquad 3.$$

The map $\mathcal{M}$ will generally be referred to as a transfer map.

2.3 *Symplectic Condition*

Suppose small changes are made in the initial conditions z^i. These small changes will induce corresponding small changes in the final conditions z^f. The relation between these small changes in the initial and final conditions can conveniently be described in terms of the Jacobian matrix M of partial derivatives given by the expression

$$M_{ab}(z^i) = \partial z_a^f / \partial z_b^i. \qquad 4.$$

Here the matrix $M(z^i)$ has been labeled by the quantity z^i to indicate that in the general case $M(z^i)$ depends on the trajectory in question.

Next, let J be a $2n \times 2n$ matrix defined by the equation

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \qquad 5.$$

Here each entry in J is an $n \times n$ matrix, I denotes the $n \times n$ identity matrix, and all other entries are zero.

Now suppose that the relation between z^i and z^f is the result of following trajectories that are governed by Hamilton's equations of motion. Such is the case for charged-particle optics (provided synchrotron radiation effects

are ignored) since charged-particle motion in electromagnetic fields can be described in Hamiltonian form. Then it can be shown that the Jacobian matrix (Equation 4) must satisfy the matrix relations

$$\tilde{M}(z^i) J M(z^i) = J. \qquad 6.$$

Here $\tilde{M}$ denotes the transpose of M.

Mathematically speaking, Equation 6 is the condition that M be a *symplectic* matrix. [For the reader interested in more detail, much of the mathematical background for this paper may be found in (22).] Correspondingly, when a map $\mathcal{M}$ has a Jacobian matrix M that is symplectic at all points, the map itself is said to be a *symplectic* map. As shown in (22), a symplectic map is essentially the same thing as a canonical transformation.

Several observations are pertinent at this point. First, Equation 6 holds for all z^i. That is, although the matrix $M(z^i)$ in general depends on z^i, the particular combination $\tilde{M}JM$ must in fact be independent of z^i. (The right-hand side of Equation 6 is the constant matrix J.) Consequently, symplectic maps are severely restricted. Second, Equation 6 is nonlinear. Thus, the restrictions are nonlinear. Finally, when these restrictions are imposed on the Taylor expansion (Equation 2), one finds that the coefficients R, T, U, etc are strongly interrelated by a large number of nonlinear conditions. Thus the quantities R, T, U, etc are far from independent and are nor always the most useful way of describing a transfer map. As an example of these restrictions, the Taylor expansion cannot in general be truncated without violating the symplectic condition.

2.4 *Symplectic Matrices and the Symplectic Group*

Suppose M is a symplectic matrix. Then it can be shown that M^{-1} exists and also is a symplectic matrix. Next, suppose that M_1 and M_2 are symplectic matrices. Then, the product $M_1 M_2$ is also a symplectic matrix. Finally, it is easily checked that the identity matrix is symplectic. These three properties show that symplectic matrices form a group (22). This group, called the symplectic group, is often referred to in the mathematics literature as the group $Sp(2n)$.

Let S by a symmetric $2n \times 2n$ matrix. Consider the matrix M defined in terms of S by the (exponential series) relation

$$M = \exp(JS) = \sum_{m=0}^{\infty} (JS)^m / m!. \qquad 7.$$

Then M is a symplectic matrix. Conversely, it can be shown that if M is a symplectic matrix, then it can be written in the form of Equation 7. Strictly

speaking, this is true only if M is sufficiently near the identity. In the general case, two exponential factors are required (see 22).

2.5 *Definition of Lie Algebras and Lie Groups*

Loosely speaking, algebra has to do with addition and multiplication. In mathematical parlance, an algebra is defined to be a linear vector space (thus providing for addition) supplemented by some rule for multiplying any two vectors to yield a third vector. Naturally, there are certain properties, such as the distributive property, that are required of the multiplication rule in order for it to be compatible with the linear vector space structure.

An algebra is called a Lie algebra if the multiplication rule satisfies two additional properties. Specifically, suppose x and y are any two vectors (elements in the algebra), and suppose their product is denoted by the customary symbols $[x, y]$. Then the multiplication rule must have the two properties

$$[x, y] = -[y, x] \text{ (antisymmetry)}, \tag{8a}$$

$$[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0 \text{ (Jacobi condition)}. \tag{8b}$$

In this context, the product symbol [,], often referred to as the Lie product, is to be viewed abstractly, and may have several different possible concrete realizations depending on the particular Lie algebra involved.

It is a remarkable fact that every Lie algebra has associated with it a certain group. These groups are called Lie groups. Roughly speaking, these groups are gotten by "exponentiating" the Lie algebras. This concept is made more precise for our purposes in subsequent sections.

2.6 *Lie Algebra of the Symplectic Group*

Suppose that S is a $2n \times 2n$ symmetric matrix, and consider matrices B of the form

$$B = JS. \tag{9}$$

Then it is obvious that such matrices form a linear vector space. Now let B_1 and B_2 be any two matrices of the form defined in Equation 9. Consider their commutator, here denoted by $[B_1, B_2]$ and defined by

$$[B_1, B_2] = B_1B_2 - B_2B_1. \tag{10}$$

Then it is easily checked that the commutator satisfies the conditions in Equations 8a and 8b for a Lie product. Finally, it is easily verified that B_3 defined by $B_3 = [B_1, B_2]$ can be written in the same form as Equation 9.

We conclude that matrices of this form constitute a Lie algebra with the commutator playing the role of a Lie product. Moreover, from Equation 7 we see that this Lie algebra is related to the group of symplectic matrices.

In particular, the exponential of any element in the Lie algebra is a symplectic matrix, and any symplectic matrix can be written in terms of such exponentials. For this reason, the Lie algebra composed of matrices of the form in Equation 9 is called the Lie algebra of $Sp(2n)$. Conversely, $Sp(2n)$ is a Lie group.

Since a Lie algebra is a vector space, it is natural to speak of its dimension. For the symplectic group, elements of the Lie algebra are of the form in Equation 9 where S is any symmetric matrix. The dimension of the Lie algebra in this case, therefore, is just the dimension of the set of all $2n \times 2n$ symmetric matrices. This dimension is easily found to be $n(2n+1)$. In particular, for $n = 3$, the Lie algebra of $Sp(6)$ has dimension 21. Consequently, in this case there are 21 linearly independent matrices of the form shown in Equation 9, and 21 parameters are required to label 6×6 symplectic matrices.

2.7 *The Group of Symplectic Maps*

Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be two symplectic maps, and suppose that these two maps are allowed to act in succession to produce a resultant map $\mathcal{M}_3$. That is, $\mathcal{M}_3$ is the product of $\mathcal{M}_1$ and $\mathcal{M}_2$. Then, from the chain rule for differentiation, it follows that the Jacobian matrix for $\mathcal{M}_3$ is the product of the Jacobian matrices for $\mathcal{M}_1$ and $\mathcal{M}_2$. Moreover, since the Jacobian matrices for $\mathcal{M}_1$ and $\mathcal{M}_2$ are symplectic, and since symplectic matrices form a group, it follows that the Jacobian matrix for $\mathcal{M}_3$ is symplectic. Hence, $\mathcal{M}_3$ is a symplectic map.

Similarly, it can be shown that if $\mathcal{M}$ is a symplectic map, then $\mathcal{M}^{-1}$ exists and is also a symplectic map. Finally, it is evident that the identity map is a symplectic map.

It follows that the set of symplectic maps forms a group (22). We show in Section 3.6 that the group of symplectic maps is also a Lie group, and the Lie algebra associated with this group is of infinite dimension.

3. ELEMENTARY LIE ALGEBRAIC METHODS

As seen in the last two sections, one of the major problems in the theoretical treatment of magnetic optics is that of producing, parameterizing, and manipulating symplectic maps. In this section we describe how these problems may be treated using Lie algebraic methods.

3.1 *Lie Operators and Their Properties*

Let $f(z) = f(q, p)$ be some specified function of the phase-space variables z. Associated with each f is a Lie operator that we denote by the symbol $:f:$. The Lie operator $:f:$ is a differential operator defined by the rule

$$:f: \overset{\text{def}}{=} \sum_{j=1}^{n} (\partial f/\partial q_j)(\partial/\partial p_j) - (\partial f/\partial p_j)(\partial/\partial q_j). \tag{11.}$$

In particular, if $:f:$ acts on any phase-space function g, one finds the result

$$:f:g = \sum_{j=1}^{n} (\partial f/\partial q_j)(\partial g/\partial q_j) - (\partial f/\partial p_j)(\partial g/\partial q_j) = [f,g]. \tag{12.}$$

Here (unlike the notation of Section 2.5) the bracket $[,]$ denotes the familiar Poisson bracket operation of classical mechanics (23).

Powers of $:f:$ are defined by taking repeated Poisson brackets. For example $:f:^2$ is defined by the relation

$$:f:^2 g = [f,[f,g]]. \tag{13.}$$

Finally, $:f:$ to the zero power is defined to be the identity operator,

$$:f:^0 g = g. \tag{14.}$$

At this point a few observations are worth making. Consider the set of all phase-space functions $f(z)$. They evidently form a linear vector space. (Any linear combination of two such functions is again a function.) Also, the Poisson bracket operation satisfies the relations in Equations 8, and hence can be viewed as a Lie product. It follows that the set of all phase-space functions forms a Lie algebra. Moreover, this Lie algebra is of infinite dimension since the vector space of functions defined on phase space is of infinite dimension.

Next consider the set of all Lie operators $:f:$. They too form a linear vector space since we can define linear combinations of Lie operators by the rule $a:f:+b:g: = :af+bg:$. Also, consider the commutator of two Lie operators, here denoted by $\{,\}$ and defined by

$$\{:f:,:g:\} = :f::g:-:g::f:. \tag{15.}$$

As seen before, the commutator satisfies the conditions for a Lie product. Finally, it can be shown that the commutator of two Lie operators is again a Lie operator. Specifically, as a result of the Jacobi identity (condition) for Poisson brackets, one has the relation

$$\{:f:,:g:\} = :[f,g]:. \tag{16.}$$

It follows that the set of all Lie operators is also an infinite-dimensional Lie algebra. Moreover, the Lie product (commutator) of any two Lie operators can be computed in terms of the Poisson bracket of their associated functions.

3.2 *Lie Transformations and Their Properties*

Since powers of $:f:$ have been defined, it is also possible to deal with power series in $:f:$. Of special importance is the power series $\exp(:f:)$. This object is called the Lie transformation associated with $:f:$. The Lie transformation is also an operator and is formally defined by the exponential series

$$\exp(:f:) = \sum_{m=0}^{\infty} :f:^m/m!. \tag{17.}$$

In particular, the action of $\exp(:f:)$ on any function g is given by the rule

$$\exp(:f:)g = g+[f,g]+[f,[f,g]]/2!+\cdots. \tag{18.}$$

Lie transformations have several remarkable properties, and in many ways seem to lead lives of their own. Two of these properties are of use for subsequent discussion. The first, which may be viewed as an exchange rule, is the relation

$$\exp(:f:)\exp(:g:) = \exp(:g:)\exp(:\exp(:-g:)f:). \tag{19.}$$

The second is the Baker-Campbell-Hausdorff theorem for combining exponents. In the present context it takes the form

$$\begin{aligned}\exp(:f:)\exp(:g:) = \exp(:f:+:g: \\ +(1/2)\{:f:,:g:\}+(1/12)\{:f:,\{:f:,:g:\}\} \\ +(1/12)\{:g:,\{:g:,:f:\}\}+\cdots).\end{aligned} \tag{20.}$$

One of the remarkable features of Equation is that only Lie operators and commutators of Lie operators appear in the exponent on the right-hand side. Consequently, by using Equation 16, we may rewrite Equation 20 in the form

$$\exp(:f:)\exp(:g:) = \exp(:h:), \tag{21a}$$

with h given by the expression

$$h = f+g+(1/2)[f,g]+(1/12)[f,[f,g]]+(1/12)[g,[g,f]]+\cdots. \tag{21b.}$$

3.3 *Production of Symplectic Maps by Lie Transformations*

Suppose $f(z^i)$ is any function of the initial phase-space variables z^i. Consider a set of final phase-space variables z^f defined by the rule

$$z_a^f = \exp(:f:)z_a^i, \qquad (a = 1,2,\ldots,2n). \tag{22.}$$

It can be shown that the relation between z^i and z^f given by Equation 22

is a symplectic map. Upon combining Equations 3 and 22, we can write the symplectic map $\mathcal{M}$ in the operator form

$$\mathcal{M} = \exp(:f:). \tag{23.}$$

What we have learned is that Lie transformations produce an endless supply of symplectic maps.

3.4 *Simple Examples*

This section describes three simple examples of symplectic maps produced by Lie transformations. These examples are important for subsequent sections. In this section they are applied to a two-dimensional phase space with coordinates q,p. However, they have obvious generalizations to higher dimensions.

First, consider the case in which the function f is of the form

$$f = -(l/2)p^2. \tag{24.}$$

Here l is a parameter whose significance becomes apparent below. Simple calculation gives the result

$$:f:p = 0, \qquad :f:^2p = 0, \qquad \text{etc.} \tag{25a.}$$

$$:f:q = -(l/2)[p^2,q] = lp, \qquad :f^2q = :f::f:q = l:f:p = 0, \qquad \text{etc.} \tag{25b.}$$

Now apply these results to evaluate Equation 22 with the aid of Equations 17 and 18. So doing gives the relations

$$q^f = \exp\{-(l/2):(p^i)^2:\}q^i = q^i + lp^i, \tag{26a.}$$

$$p^f = \exp\{-(l/2):(p^i)^2:\}p^i = p^i. \tag{26b.}$$

Examination of Equations 26 shows that the map $\mathcal{M} = \exp(:f:)$ with f given by Equation 24 is the transfer map for simple transit (a drift in accelerator terminology) over a distance l.

Next, consider the case in which the function f is of the form

$$f = -(w/2)(q^2+p^2). \tag{27.}$$

Here again w is a parameter. In this case, repeated application of the operator $:f:$ as required by Equation 22 gives an infinite series. However, the series can easily be summed to give the result

$$q^f = \exp\{-(w/2):(q^i)^2+(p^i)^2:\}q^i = q^i \cos w + p^i \sin w, \tag{28a.}$$

$$p^f = \exp\{-(w/2):(q^i)^2+(p^i)^2:\}p^i = -q^i \sin w + p^i \cos w. \tag{28b.}$$

Examination of Equations 28 shows that the map $\mathcal{M} = \exp(:f:)$ with f given by Equation 27 produces a rotation in phase space (a phase advance in accelerator terminology) by an amount w.

As a final example, consider the case in which the function f is of the form

$$f = (s/3)q^3. \tag{29.}$$

Here again s is a parameter. The reader is invited to derive in this case the relations

$$q^f = q^i, \tag{30a.}$$

$$p^f = p^i + s(q^i)^2. \tag{30b.}$$

These are the relations expected for the nonlinear action of a sextupole in the thin-lens (kick) approximation.

3.5 *Factorization Theorem*

Section 3.3 described how Lie transformations can be used to produce symplectic maps, and Section 3.4 gave three simple examples.

Conversely, suppose $\mathcal{M}$ is any symplectic map having a Taylor series expansion of the form seen in Equation 2. Then $\mathcal{M}$ can be written uniquely in the factored product form

$$\mathcal{M} = \exp(:f_1:)\exp(:f_2:)\exp(:f_3:)\exp(:f_4:)\cdots. \tag{31.}$$

Here each function f_m is a homogeneous polynomial of degree m in the variables z^i (24; see also 22, 25, 26).

By definition, a knowledge of $\mathcal{M}$ is equivalent to a knowledge of the relation between the initial conditions z^i and the final conditions z^f. And, according to the factorization theorem (Equation 31), a knowledge of $\mathcal{M}$ amounts to determining certain homogeneous polynomials f_1, f_2, f_3, f_4, etc. This is a key result.

When applied to charged-particle optics, the factorization theorem indicates that the effect of any collection of elements can be characterized by a set of homogeneous polynomials. Moreover, unlike the terms K_a, R_{ab}, T_{abc}, etc, in the Taylor series (Equation 2), the polynomials f_m are all independent. That is, any set of polynomials when employed in Equation 31 produces a symplectic map. Conversely any symplectic map can be written uniquely in the form of Equation 31. Finally, the product (Equation 31) can be truncated at any stage, and the result is still a symplectic map.

For example, the Lie algebraic description of a transfer map through fifth order requires the polynomials f_1 through f_6. The specification of these polynomials (in six variables) requires 923 coefficients. By contrast, the specification of the Taylor coefficients through this order requires 2766

coefficients, and even more coefficients if symmetry under the exchange of indices is not exploited. Thus, the use of Lie algebraic methods requires considerably less computer storage, and should in principle also enhance computational speed.

Thus, from a Lie algebraic perspective, the fundamental problem of charged-particle optics is to study what polynomials correspond to various optical elements, to study what polynomials result from concatenating various optical elements, and to study what polynomials correspond to various desired optical properties.

Each factor in Equation 31 has a direct physical interpretation. It can be shown that the factor $\exp(:f_1:)$ reproduces the constant terms K_a in the Taylor expansion (Equation 2), and thus produces a simple translation in phase space. Next, as the first two examples in Section 3.4 illustrate, the factor $\exp(:f_2:)$ produces linear transformations corresponding to the linear matrix (paraxial optics) coefficients R_{ab}. The last example in Section 3.4 illustrates that the factor $\exp(:f_3:)$ produces second (and possibly higher) order aberration terms corresponding to the coefficients T_{abc}, U_{abcd}, etc. Similarly, the factor $\exp(:f_4:)$ produces third (and possibly higher) order aberration terms corresponding to the coefficients U_{abcd}, etc.

Put another way, in terms of beam-line components, we may say that $\exp(:f_1:)$ describes magnet misplacement errors and dipole powering errors; $\exp(:f_2:)$ describes linear transport in drifts, dipoles, and quadrupoles; $\exp(:f_3:)$ describes sextupole effects; $\exp(:f_4:)$ describes octupole effects, etc. Finally, it can be shown that the factors in Equation 31 act from left to right. That is, this factorization decomposes a general symplectic map into a phase-space translation, followed by a linear transformation, followed by a second-order transformation, followed by a third-order transformation, etc.

3.6 *Lie Algebra of the Group of Symplectic Maps*

Section 3.1 showed that the set of Lie operators forms a Lie algebra. Moreover, according to Sections 3.3 and 3.5, the exponential of a Lie operator is a symplectic map, and any symplectic map can be expressed in terms of such exponentials. It follows that the group of symplectic maps is a Lie group, and its Lie algebra is the set of Lie operators. As we have seen, this Lie algebra is infinite dimensional.

Because the Lie algebra of Lie operators is infinite dimensional, the specification of a symplectic map generally requires an infinite number of parameters. This is an awkward situation for human beings and computers, which can only work with a finite number of quantities (and often only with finite precision).

An optimistic perspective on the experimental and theoretical situation might be stated as follows: We know that a beam transport system, accelerator, storage ring, or any portion thereof may be described by a symplectic transfer map. However, because we cannot measure or control electromagnetic fields exactly, we are unsure of and unable to control exactly what this map is. Also, since it is impossible to perform computations with an infinite number of variables and to infinite precision, it is necessary to develop various approximation schemes. Thus, we are able to study computationally (and probably theoretically) the detailed properties of only a subset of all symplectic maps. The hope is that if two symplectic maps are in some sense nearly the same, then their behavior and their long-term effects are nearly the same. If this were not true from an experimental standpoint, then it would be impossible to build satisfactory storage rings, etc. If this were not true from a theoretical standpoint, then it would be impossible to design storage rings etc with any assurance that their actual performance would be satisfactory.

Note that ray-trace calculations involving kick approximations are also not exact; consequently some such argument as that just made is also required to justify their use.

3.7 *Truncation Methods*

As just described, it is necessary to develop some sort of approximation scheme to treat symplectic maps in a practical way. In this section we sketch the outline of a truncation scheme that maintains a Lie algebraic structure (25, 26). We show in the next section that the rules for multiplying symplectic maps can be expressed entirely in Lie algebraic terms. Thus, if the truncation scheme maintains a Lie algebraic structure, it follows that maps may either be truncated and then multiplied, or multiplied and then truncated. The results from both procedures are guaranteed to be the same.

Consider entities f_{lm} of the form

$$f_{lm} = \varepsilon^l f_m. \tag{32.}$$

Here f_m is a homogeneous polynomial of degree m, and ε is a small parameter. Next, assign to each f_{lm} an integer, called the rank of f_{lm}, by the rule

$$\text{rank } f_{lm} = l+m. \tag{33.}$$

Then, it is easily verified that one has the relation

$$\text{rank}\,[f_{jk}, f_{lm}] = (\text{rank } f_{jk}) + (\text{rank } f_{lm}) - 2. \tag{34.}$$

Next consider all f_{lm} with rank ≥ 2. In view of Equation 34, these entities form an infinite-dimensional Lie algebra under Poisson bracketing. Now

consider what happens if one arbitrarily decides to discard all entities f_{lm} whose rank exceeds some integer N, and to discard all Poisson brackets whose results have rank exceeding N. Then it is easy to verify that what remains forms a finite-dimensional Lie algebra. (In technical terms, entities whose rank exceeds N form a Lie algebraic ideal; the decision to discard an ideal is equivalent to passing to the quotient Lie algebra. Finally, the exponentials of elements in the quotient Lie algebra form a quotient Lie group.) For the concepts of ideals, quotient algebras, and quotient groups, see (27).

Correspondingly, in view of Equation 16, this truncation scheme can be carried over to the associated set of Lie operators simply by ignoring all $:f_{lm}:$ for which the rank of f_{lm} lies outside the range $N \geq \text{rank} \geq 2$. Thus, one may also produce in this way a finite-dimensional Lie algebra of Lie operators.

What does this have to do with magnetic optics? First, according to Section 3.5, the polynomials f_m describe aberrations of order $(m-1)$; and the decision to ignore all entities whose rank exceeds N implies the neglect of all aberrations whose order exceeds $(N-1)$. Correspondingly, the factored product (Equation 31) is truncated at $\exp(:f_N:)$.

Second, suppose one makes the natural assumption that one is interested only in systems for which misalignment, misplacement, and mispowering errors are small. Then, it is natural to consider the entity εf_1, rather than f_1, where ε is a measure of the smallness of the errors under consideration. Now all Lie algebraic calculations can proceed with all entities having a rank satisfying the condition $N \geq \text{rank} \geq 2$. All decisions as to what to neglect and what to retain are made on the basis of rank. Finally, when the calculation is complete, one recognizes that the use of rank and the ε parameter was, in fact, merely an ordering technique for making expansions both in aberration order and in powers of the errors. One then sets $\varepsilon = 1$. When this is done, the burden of smallness is borne by the various f_1 polynomials themselves.

In summary, we have learned that the neglect of aberrations beyond any fixed order is consistent with the underlying group structure of symplectic maps. Moreover, we have seen that it is possible to have a self-consistent Lie algebraic treatment of optical systems with errors, provided these errors are small.

3.8 *Concatenation Formulas*

Consider a transport line, accelerator, storage ring, etc that is composed of several successive elements. Suppose that the transfer map for each individual element is known, and that what is desired is the transfer map for the entire system. This total transfer map will be the product of the individual transfer maps. Evidently what is needed is a procedure for multiplying any two transfer maps to yield a third transfer map.

Suppose $\mathcal{M}_f$ and $\mathcal{M}_g$ are two symplectic transfer maps expressed in factored product form:

$$\mathcal{M}_f = \exp(:f_1:)\exp(:f_2:)\exp(:f_3:)\ldots, \tag{35.}$$

$$\mathcal{M}_g = \exp(:g_1:)\exp(:g_2:)\exp(:g_3:)\ldots. \tag{36.}$$

Let $\mathcal{M}_h$ be the product of $\mathcal{M}_f$ and $\mathcal{M}_g$,

$$\mathcal{M}_h = \mathcal{M}_f\mathcal{M}_g. \tag{37.}$$

Then, by the group property of symplectic maps, $\mathcal{M}_h$ must also be a symplectic map. Consequently, by the factorization theorem, it must be expressible in the factored product form

$$\mathcal{M}_h = \exp(:h_1:)\exp(:h_2:)\exp(:h_3:)\ldots. \tag{38.}$$

Thus, given the polynomials $f_1, f_2, f_3, \ldots$ and $g_1, g_2, g_3, \ldots$, the problem is to find the polynomials $h_1, h_2, h_3, \ldots$.

This problem can be solved with the aid of the exchange rule (Equation 19) and the Baker-Campbell-Hausdorff theorem (Equation 21). The required calculations are too lengthy to be reproduced here, and we must be content simply to sketch results. Moreover, although results have been obtained through terms of rank 6 (as defined in Section 3.7) and implemented through this rank in the program MARYLIE 5.1, these results themselves are too long to be listed here (26, 28). Therefore, we present results only through rank 4. This is sufficient to illustrate most essential features. Also, these results are useful in their own right, and have been implemented in the program MARYLIE 3.1.

To clarify nomenclature, the program MARYLIE 3.1 works with transfer maps of the form $\mathcal{M} = \exp(:f_1:)\exp(:f_2:)\exp(:f_3:)\exp(:f_4:)$ while MARYLIE 3.0 works only with maps of the form $\mathcal{M} = \exp(:f_2:)\exp(:f_3:)\exp(:f_4:)$. Thus, both programs work through third order, but MARYLIE 3.0 does not treat misalignment, misplacement, and mispowering errors. MARYLIE 5.1 works with maps of the form $\mathcal{M} = \exp(:f_1:)\ldots\exp(:f_6:)$. Thus, it handles errors and works through fifth order.

The first step in computing the polynomials $h_1, h_2, \ldots$ is to write out Equation 38 in the form

$$\mathcal{M}_h = \exp(:f_1:)\exp(:f_2:)\exp(:f_3:)\ldots\exp(:g_1:) \times \exp(:g_2:)\exp(:g_3:)\ldots. \tag{39.}$$

The next (and most difficult) step is to move the factor $\exp(:g_1:)$ to the left in such a way that all the terms coming before the second line of

Equation 39 are rewritten in standard factored product form. When this is done one finds an expression of the form

$$\mathcal{M}_h = \exp(:k_1:)\exp(:k_2:)\exp(:k_3:)\ldots \times \exp(:g_2:)\exp(:g_3:)\ldots. \quad 40.$$

Explicitly, through terms of rank 4, one finds the results

$$k_1 = f_1 + \exp(:f_2:)(g_1 + :g_1:^2 f_3/2 - :g_1:^3 f_4/6 - [:g_1:f_3, :g_1:^2 f_3]/4), \quad 41a.$$

$$\exp(:k_2:) = \exp(:f_2:)\exp\{:(-:g_1:f_3 + :f_3::g_1:^2 f_3/4 + :g_1:^2 f_4/2):\}, \quad 41b.$$

$$k_3 = f_3 - :f_3::g_1:f_3/2 - :g_1:f_4, \quad 41c.$$

$$k_4 = f_4. \quad 41d.$$

The last step is to manipulate the factors in Equation 40 to bring the net result into the factored product form (Equation 38). When this is done, one finds the final result

$$h_1 = k_1, \quad 42a.$$

$$\exp(:h_2:) = \exp(:k_2:)\exp(:g_2:), \quad 42b.$$

$$h_3 = k_3^{\mathrm{tr}} + g_3, \quad 42c.$$

$$h_4 = [k_3^{\mathrm{tr}}, g_3]/2 + k_4^{\mathrm{tr}} + g_4. \quad 42d.$$

Here the transformed quantities k_m^{tr} are given by the relations

$$k_m^{\mathrm{tr}} = \exp(:-g_2:)k_m. \quad 43.$$

Several comments are now in order. First, as has been seen earlier, Lie transformations generated by quadratic polynomials correspond to linear matrix transformations. Thus, for such maps, it is simplest to express their product in a form analogous to matrix multiplication as in Equations 41b and 42b, rather than as rules for combining exponents. Second, notice that Equation 41c for k_3 contains terms involving g_1 and f_4. This is an example of a nonlinear "feed-down" effect. It shows, for example, that a misplaced octupole can produce sextupole-like effects. Equation 41b exhibits even more complicated nonlinear feed-down effects. Finally, notice that Equation 42d for h_4 contains terms involving k_3 and g_3. This is an example of "cross-coupling" between nonlinearities to produce still higher order nonlinear effects. It shows, for example, that the actions of two sextupoles can combine to produce octupole-like effects.

3.9 *Computation of Maps*

As described in Section 2.3, the evolution of a system governed by Hamilton's equations of motion produces a symplectic transfer map. The purpose of this section is to make some remarks about how, given the Hamiltonian, this map may be computed.

In the construction of accelerators and most other charged-particle beam transport systems, it is customary to employ a modular approach. That is, these systems are composed of several individual elements each of which has a separate function. Lie algebraic methods are ideally suited (although not restricted) to such an approach. For, if the transfer maps for individual elements are known, as in Section 3.8, then the transfer map for a composite system can be obtained by concatenation. Thus, when using Lie algebraic methods, it is convenient to extract all relevant information from the Hamiltonian once and for all at the beginning, and to work from then on only with transfer maps.

Suppose one wishes to compute the transfer map for some beam-line element. It is convenient to begin with the "design orbit" for that element. In an idealized dipole, the design orbit is a portion of a circular arc. In an idealized quadrupole, sextupole, octupole, etc, the design orbit is a straight line. In a real element (for example a dipole with fringe fields or an rf cavity having curved field lines), the determination of the design orbit generally requires numerical integration.

Once the design orbit has been found, one introduces new variables that measure deviations from the design orbit, and then seeks to express the transfer map in terms of these variables. When this is done, the transfer map $\mathcal{M}$ obeys an equation of motion of the form

$$\dot{\mathcal{M}} = \mathcal{M}:-H:. \quad 44.$$

Here H is the Hamiltonian (expressed in deviation variables) that describes motion in the beam-line element under study, and the dot indicates differentiation with respect to some independent variable that may be the time, but is often conveniently taken to be some coordinate that describes the progress of a trajectory through the beam-line element.

To proceed further, it is useful to write the transfer map in factorized product form, as described in Section 3.5. When this is done, Equation 44 gives equations of motion for the R matrix corresponding to the factor $\exp(:f_2:)$, and equations of motion for the various polynomials f_3, f_4, etc (29). (The f_1 polynomial is absent because in the present discussion $\mathcal{M}$ has been defined in terms of deviation variables. That is, by construction, $\mathcal{M}$ in this case maps the origin of phase space into itself.) Furthermore, one finds that the equations for a given f_m involve only terms in H of degree

m and lower. Thus, the neglect of all aberrations whose order exceeds $(N-1)$, as discussed in the Section 3.7, is equivalent to discarding all terms in the Hamiltonian whose degree exceeds N.

In the case of an ideal beam-line element (for which the fields do not depend upon how far the trajectory has progressed within the element and H consequently does not depend on the independent variable), the equations of motion for R, f_3, f_4, etc can be solved analytically. This has been done for the common ideal beam-line elements, and the results form the basis for a library of transfer maps for these elements in the various MARYLIE codes. The calculation of transfer maps through third order is described in (30). These maps are used in MARYLIE 3.0 and MARYLIE 3.1. (Usually these calculations were done with the aid of symbolic manipulators such as MACSYMA and SMP. MACSYMA is a product of Symbolics Corporation. SMP is a product of Inference Corporation.) Eventually these calculations will have to be extended to fifth order for use in MARYLIE 5.1.

In the case of a real beam-line element, including the effects of fringe fields etc, the equations of motion for $R, f_3, f_4, \ldots$ can easily be integrated numerically. This approach is implemented in a family of GENMAP codes. These codes take as input electric and magnetic field data (either computed or measured) and provide as output both the design orbit and the map $\mathcal{M}$ about the design orbit in factored product form. This map may then be used in subsequent calculations in other Lie algebraic codes (31, 33). There are now versions of GENMAP called GENDIP 3.0 and GENREC 3.0 that routinely handle dipoles and REC (rare earth cobalt) quadrupoles through third order, including fringe-field effects. The use of the code SCB (an independent realization of GENMAP for treating dipoles through third order) for the design of compact storage rings with superconducting bends is described in the papers of Moser et al (33a). GENREC 5.0, a program for handling REC quadrupoles through fifth order, is currently being tested (F. Neri, report in preparation, 1988). In principle, GENMAP could work to arbitrarily high order provided that one had a suitable power series expansion of the Hamiltonian H about the design orbit. One convenient way of obtaining such expansions is through the use of differential algebra (see 32).

The discussion so far has been restricted to elements that are perfectly aligned, positioned, and powered. As mentioned earlier, for such elements there are no $\exp(:f_1:)$ terms in the corresponding maps. When a properly powered element is misaligned and/or mispositioned, the complete transfer map (including the effect of these errors) can be obtained from the map for a perfectly aligned and positioned element simply by pre- and post-multiplying this map by certain other "matching" maps. These matching

maps, which describe rigid-body translations and rotations, have been worked out in detail. In general, they involve $\exp(:f_1:)$ factors. Similarly, if the element is mispowered as well, there is again a standard procedure for computing an analogous set of matching maps. Finally, it can be shown that the transfer maps for the standard correction elements, such as steering magnets, also involve $\exp(:f_1:)$ factors. Thus these factors can be used to compensate for the $\exp(:f_1:)$ factors arising from errors. All these procedures have been incorporated into the code MARYLIE 3.1 through third order, and the code MARYLIE 5.1 through fifth order (25, 26, 28).

In summary, we have presented some of the highlights of well-established procedures for computing the transfer maps for individual elements, both idealized and real, and both without and with alignment, positioning, and powering errors. These maps can then be combined using the concatenation procedures described in Section 3.8 to obtain the transfer map for any complete system or any portion thereof.

4. ADVANCED LIE ALGEBRAIC METHODS

The previous section described what may be called elementary Lie algebraic methods. These methods are basic to all Lie algebraic calculations and are sufficient for various applications such as ray tracing and aberration correction and control. The purpose of this section is to describe some advanced Lie algebraic methods that are useful in the construction of invariants and the analysis of transfer maps.

4.1 *Structure Constants*

Consider an arbitrary Lie algebra. Since a Lie algebra is a vector space, it must have a basis. Suppose some basis is selected, and let the various basis elements be denoted as B_1, B_2, B_3, etc.

Now consider the Lie product of any two basis elements. Since the Lie product is again an element in the Lie algebra, it must be expandable in terms of the basis elements. Consequently, there must be a set of coefficients c_{ijk}, called structure constants, such that one has the relations

$$[B_i, B_j] = \sum_k c_{ijk} B_k. \tag{45.}$$

4.2 *Killing Form and Metric Tensor*

Since a Lie algebra is a vector space, it is reasonable to consider the possibility of introducing some kind of scalar product. This can be done in a natural way with the aid of the structure constants.

Suppose B_i is any basis element in the Lie algebra. For each B_i we define a matrix b_i by the rule

$$(b_i)_{jk} = c_{ijk}. \tag{46.}$$

In the Lie algebraic literature, the matrix b_i is often referred to as the adjoint representation of B_i, and is often written as $b_i = \mathrm{ad}(B_i)$.

Now let B_i and B_j be any two basis elements in the Lie algebra. With the aid of the concepts just introduced, we define the scalar product of B_i and B_j, denoted by (B_i, B_j), by the relation

$$(B_i, B_j) = \mathrm{trace}\,(b_i b_j). \tag{47.}$$

The right-hand side of Equation 47 is called the Killing form. For a discussion of structure constants and the Killing form see, for example, (34).

It is convenient to view the collection of numbers represented in Equation 47 as the elements of a symmetric tensor, called the metric tensor. That is, we define entries g_{ij} by the rule

$$g_{ij} = (B_i, B_j) = \mathrm{trace}\,(b_i b_j). \tag{48.}$$

For certain Lie algebras, the metric tensor is invertible. In the invertible case, it is also useful to define a metric tensor g^{ij} with superscript indices by the rule

$$g^{ij} = (g^{-1})_{ij}. \tag{49.}$$

For those interested in more detail, we note that the Killing form (metric tensor) is invertible if an only if the Lie algebra is semisimple (35). The Lie algebras $Sp(2n)$ are semisimple, but the quotient Lie algebras of Section 3.7 are not.

4.3 *Conjugacy Classes and Normal Forms*

Let $\mathcal{M}$ and $\mathcal{N}$ be any two symplectic maps. Suppose a third symplectic map $\mathcal{A}$ exists such that $\mathcal{M}$, $\mathcal{N}$, and $\mathcal{A}$ are connected by the relation

$$\mathcal{M} = \mathcal{A}^{-1}\mathcal{N}\mathcal{A}. \tag{50.}$$

Then $\mathcal{M}$ is said to be conjugate to $\mathcal{N}$.

Note that Equation 50 can be written in the equivalent form

$$\mathcal{N} = \mathcal{A}\mathcal{M}\mathcal{A}^{-1}. \tag{51.}$$

Also, since $\mathcal{A}$ is a symplectic map, so is $\mathcal{A}^{-1}$. It follows that if $\mathcal{M}$ is conjugate to $\mathcal{N}$, then $\mathcal{N}$ is also conjugate to $\mathcal{M}$. Maps that are conjugate to each other are said to belong to the same conjugacy class.

There are a variety of theorems that state under what conditions two maps $\mathcal{M}$ and $\mathcal{N}$ are conjugate. Some of these theorems are described and applied in Section 6. If $\mathcal{N}$ takes a particularly simple form, it is referred to as a normal form. Thus, given $\mathcal{M}$, one subject of interest is the exploration of how simple the map $\mathcal{N}$ can be made by a suitable choice of $\mathcal{A}$. Note that the process of finding a normal form is the nonlinear generalization of the linear problem of matrix diagonalization. Finally, it is evident that two maps belong to the same conjugacy class if and only if they have the same normal form.

5. ELEMENTARY APPLICATIONS

In this section we describe briefly some of the applications of mostly elementary Lie algebraic methods to some problems in charged-particle beam dynamics.

5.1 *Single-Particle Transport*

To compute single-particle transport, it is necessary to evaluate Equation 3 with $\mathcal{M}$ can easily be evaluated since, as described in Section 3.5, the factor $\exp(:f_1:)$ simply produces a phase-space translation, and the factor $\exp(:f_2:)$ produces a linear transformation that can be implemented simply in terms of the associated matrix R. The effect of the remaining product of factors $\exp(:f_3:)\exp(:f_4:)\ldots$ is somewhat more difficult to evaluate. Two approaches are currently available.

The first approach is to use a truncated Taylor series. For example, through third order, one may simply write

$$\exp(:f_3:)\exp(:f_4:) = (1 + :f_3: + :f_3:^2/2! + \ldots)(1 + :f_4: + \ldots)$$
$$\approx 1 + :f_3: + :f_3:^2/2! + :f_4:. \tag{52.}$$

That is, all terms that would produce contributions of order higher than three are simply ignored. (It is easily verified that the expansion in Equation 52 is equivalent to the Taylor series in Equation 2 truncated beyond terms of degree three.) This method is adequate for single-pass systems such as beam lines, spectrometers, final focus assemblies, spot forming systems, and telescopes. It has the advantage of high computational speed. For example, when running on a CRAY X-MP, third-order MARYLIE can carry out more than 4000 such ray traces per second. With proper attention to the use of vector processing, this speed could undoubtedly be made even greater.

Although the truncated Taylor series method is fast, it has the disadvantage (described in Section 2.3) that it generally violates the symplectic condition. This violation is usually not important for studying single-pass

systems. However, it can be very important for long-term particle-tracking simulations such as following 10^6 to 10^8 turns in a storage ring.

One way to overcome this problem is to represent the action of the product of factors $\exp(:f_3:)\exp(:f_4:)\ldots$ by means of a generating function. Consider a function F of initial q's and final p's written in the form

$$F(q^i,p^f) = q^i\cdot p^f + P(q^i,p^f), \tag{53.}$$

where P is a polynomial yet to be determined. Then, use of the standard relations

$$p^i = \partial F/\partial q^i = p^f + \partial P/\partial q^i, \tag{54a.}$$

$$q^f = \partial F/\partial p^f = q^i + \partial P/\partial p^f \tag{54b.}$$

is guaranteed to produce a symplectic transformation for any choice of P. Finally, the polynomial P is chosen in such a way that this transformation agrees with that given by $\exp(:f_3:)\exp(:f_4:)\ldots\exp(:f_N:)$ through terms of degree $(N-1)$. Indeed, it can be shown that if P is required to contain terms only of degree N and lower, then P is completely determined by a knowledge of the polynomials $f_3, f_4, \ldots, f_N$ (36). Note that in this application the generating function F is used to describe only the map $\exp(:f_3:)\exp(:f_4:)\ldots$. This map is always near the identity map, and therefore only one kind of generating function is ever required. For a discussion of symplectification of second-order codes ($N = 3$), see (37).

A complication of this method is that the relations in Equations 54 are implicit. This difficulty is overcome in the context of ray tracing by means of Newton's method. Suppose Equation 54a is rewritten in the form

$$p^f = p^i - \partial P/\partial q^i = p^i - P_q(q^i,p^f). \tag{55.}$$

Then, given the numerical values of q^i, p^i, the value of p^f is found by solving Equation 55 numerically using Newton's method. Finally, after p^f has been found, the value of q^f is obtained by evaluating Equation 54b. With careful attention to vector processing, this procedure can also be quite fast. For example, when running on a CRAY X-MP, fifth-order MARYLIE can now carry out approximately 2000 such ray traces per second (including synchrotron oscillations).

How well does all this work in practice? Figure 2 shows phase-space data equivalent to that obtained by conventional tracking methods for the Tevatron lattice with several distortion sextupoles powered to produce strong nonlinear effects. In this simulation, sixteen nonskew distortion sextupoles were powered with a current of 30 amperes. In addition, the first eight of these sextupoles were given skew components corresponding

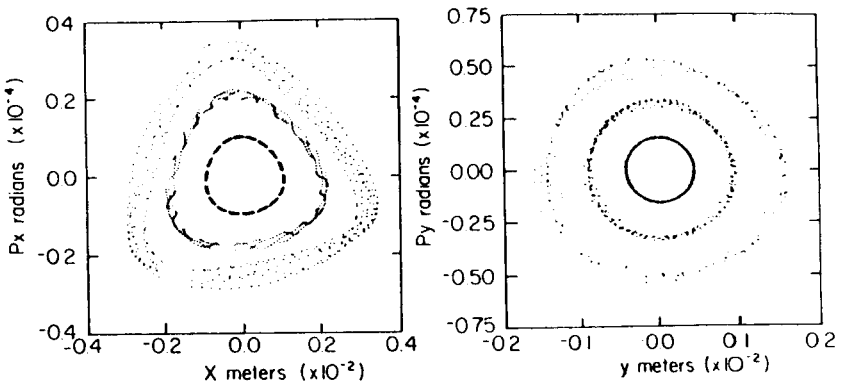


Figure 2 Horizontal (*left*) and vertical (*right*) projections of turn-by-turn Tevatron phase-space data obtained for three orbits using element-by-element tracking.

to an additional 30 A. The horizontal and vertical fractional tunes were set to 0.39 and 0.46, respectively, and first-order chromaticities were set to zero using the standard set of chromaticity-correcting sextupoles. In order to mimic conventional tracking results, MARYLIE tracking was done element by element with all sextupoles treated in the kick approximation. Three particles were followed, and phase-space data were plotted at the end of each turn for a total of 500 turns. Both horizontal and vertical (as well as temporal) betatron oscillations are excited. For a description of Fermilab Experiment E778 in which the behavior of the Tevatron with strongly powered distortion sextupoles is studied experimentally, see (38).

For comparison, Figure 3 shows phase-space data produced by fifth-

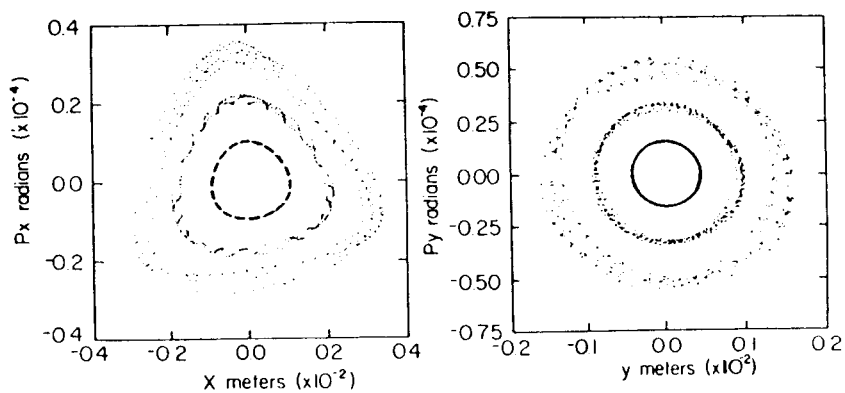


Figure 3 Horizontal (*left*) and vertical (*right*) projections of turn-by-turn Tevatron phase-space data obtained using the one-turn map through fifth order.

order MARYLIE using the full one-turn map for the Tevatron and the symplectic ray-trace procedure just described. To produce the phase-space data of Figure 3, the transfer maps for all the individual elements in the Tevatron, including the kick maps for the sextupoles, were concatenated together through fifth order to provide a one-turn map. This map was then applied repeatedly (using Equation 54) 500 times starting with the same three initial conditions used in Figure 2, and the resulting phase-space data were plotted after each application of the one-turn map.

Inspection of Figures 2 and 3 shows that, particularly for the two inner sets of data, the agreement between the two tracking procedures is excellent. Moreover, the Lie algebraic procedure is orders of magnitude faster. This is because conventional methods must track element by element through a machine, and the Tevatron has a large number of elements. By contrast, in many circumstances MARYLIE is able to track one full turn or more at a time.

A possible application of this procedure is the study of long-term orbit behavior in the proposed Superconducting Super Collider (SSC). The SSC will have a circulation time of about 1/3000 second. Thus, if the behavior of the SSC can be well approximated by a one-turn map for orbits of physical interest as experience with the nonlinearly distorted Tevatron suggests, it should be possible to use MARYLIE to compute orbits in the SSC nearly in real time. Indeed, with improved coding and faster computers, it may even be possible to compute orbits faster than real time. Thus, a direct numerical study of the long-term behavior of orbits in the SSC seems quite feasible. For a description of the SSC, see (57).

Although very advantageous whenever possible, the use of the one-turn map (or any map obtained by extensive concatenation) for tracking has to be done with care and understanding. Let $\mathcal{M}_1$ be the effective one-turn map whose results are equivalent to those obtained from element-by-element tracking, and let $\mathcal{M}_2$ be the map associated with concatenation and the use of the symplectic ray-trace procedure (Equation 54). In general the two maps $\mathcal{M}_1$ and $\mathcal{M}_2$ are not the same although, by construction, they are identical through the order of the truncation procedure. Put another way, they are represented by the same element in the quotient group. In practice, the extent to which they give the same results for orbits of physical interest must be checked by making comparisons of the type just described. That is, when tracking by this method (or, for that matter, by any other method) one must verify whenever possible assumptions of the kind described in Section 3.6.

In this context, it should be mentioned that the type of symplectification procedure employed may also make a difference. For this reason, it would be useful to have alternatives to the generating function method (Equation 54). One such alternative currently under study is the use of Cremona maps (41). For our purposes, Cremona maps are symplectic maps whose Taylor series expansions terminate. The goal would be to represent any map of the form shown in Equation 31 by a sequence of Cremona maps in such a way that their net result would agree with Equation 31 through terms of degree $N-1$. When used for tracking, the effect of the sequence of Cremona maps would be evaluated exactly.

5.2 *Transport of Moments and Moment Invariants*

The previous section briefly described single-particle transport. In some circumstances, it is useful to consider the transport of a distribution of particles in the approximation that their mutual interaction is neglected. In particular, one may be interested in how moments of the particle distribution are affected by transport. The purpose of this section is to show how such computations may be carried out directly by Lie algebraic means without ray tracing. In addition, we briefly discuss quantities that remain invariant when the transfer map has no nonlinear factors. For simplicity, we restrict our discussion to a four- or six-dimensional phase space.

Suppose $h(z)$ is the initial distribution function describing the density of particles in phase space at the entrance to some charged-particle beam system. Here as before, the symbol z denotes the collection of phase-space variables. Also, let $P_\alpha(z)$, where α is some running index, denote a complete set of homogeneous polynomials in z through terms of some fixed degree. The one can define a set of initial "moments" m_α^i by the relations

$$m_\alpha^i = \int d^6z\, h(z)\, P_\alpha(z). \tag{56.}$$

Now suppose the particle distribution is transported through the system, and suppose the single-particle action of the system is described by the map $\mathcal{M}$. Then the final distribution at the end of the system is given by $h(\mathcal{M}^{-1}z)$. Correspondingly, the final moments are given by the expressions

$$m_\alpha^f = \int d^6z\, h(\mathcal{M}^{-1}z)\, P_\alpha(z). \tag{57.}$$

Equation 57 for the final moments can be manipulated to produce a relation between initial and final moments. First, change its integration variables to give

$$m_\alpha^f = \int d^6z\, h(z)\, P_\alpha(\mathcal{M}z). \tag{58.}$$

This is possible because it can be shown from the symplectic condition in Equation 6 that the Jacobian matrix (Equation 4) has unit determinant. Next, consistent with the truncation procedure of Section 3.7 and thanks to the completeness of the P_α, one has a relation of the form

$$P_\alpha(\mathcal{M}z) = \sum_\beta D_{\alpha\beta}(\mathcal{M})\, P_\beta(z). \qquad 59.$$

The coefficients $D_{\alpha\beta}(\mathcal{M})$ may be viewed as forming a representation of the quotient group corresponding to the quotient Lie algebra associated with the truncation procedure. Finally, when Equation 59 is substituted into Equation 58, one finds

$$m'_\alpha = \sum_\beta D_{\alpha\beta}(\mathcal{M}) m'_\beta. \qquad 60.$$

Equation 60 has several interesting consequences. First, it shows that in order to transport moments, it is not necessary to perform ray traces on a large number of particles. Instead, it is only necessary to know the coefficients $D_{\alpha\beta}(\mathcal{M})$. These coefficients can be calculated for any transfer map $\mathcal{M}$ by standard Lie algebraic techniques. Indeed, one of the features of the various MARYLIE codes is the ability to transport moments in this fashion. This MARYLIE feature and its associated mathematical machinery have not yet been completely documented. For a partial description, see (33).

Second, Equation 60 shows that the various moments transform as vectors. This fact can be exploited to construct invariants when $\mathcal{M}$ is a linear transformation. For example, consider those P_α that are homogeneous of degree 2. It is obvious that they form a Lie algebra under Poisson bracketing, and it can be shown that this Lie algebra is the Lie algebra of $Sp(2n)$. Let $g^{\alpha\beta}$ (with the values of α, β restricted to those associated with quadratic polynomials) be the corresponding metric tensor with superscript indices. Then it can be shown that the quantity E_2 defined by

$$E_2 = \sum_{\alpha,\beta} g^{\alpha\beta} m_\alpha m_\beta \qquad 61.$$

is an invariant. That is, the value of E_2 is unchanged under transport as long as $\mathcal{M}$ has no nonlinear part. Specifically, in the case of a four-dimensional phase space, E_2 is given by the relation

$$E_2 = \langle x^2\rangle\langle p_x^2\rangle - \langle xp_x\rangle^2 + \langle y^2\rangle\langle p_y^2\rangle - \langle yp_y\rangle^2 + 2\langle xy\rangle\langle p_x p_y\rangle - 2\langle xp_y\rangle\langle yp_x\rangle. \qquad 62.$$

Here the angular brackets are an alternative notation for the phase-space averaging in Equation 56. The knowledgeable reader may recognize that Equation 62 is a generalization of what is called the mean square emittance to the case of four-dimensional phase space including the possibility of linear coupling between planes. The invariant E_2 was first obtained using other means (39)

From a group-theoretic perspective, one can show that the quadratic moments (the m_α corresponding to second-degree polynomials) transform according to the adjoint representation of $Sp(2n)$. Equation 61 says that the product of two such representations can be coupled "down" to produce an identity representation (invariant), with the $g^{\alpha\beta}$ acting as Clebsch-Gordan coefficients. With this in mind, one can show that for $Sp(2n)$ there are in fact n invariants made from quadratic moments. Moreover, they may be viewed as functions of n eigen-emittances. Thus, for $Sp(4)$ there is another invariant involving quadratic moments in addition to that of Equation 62, and for $Sp(6)$ there are two more. The calculation of all three invariants as well as all eigen-emittances has been implemented in the various MARYLIE codes. Unfortunately, these additional invariants require more than a page to write down and are not presented here (40, 41). Finally, one can show that it is also possible to construct invariants out of higher degree moments. They, too, transform according to certain representations of $Sp(2n)$, and certain products of them can also be coupled down to produce invariants with the aid of suitable Clebsch-Gordan coefficients (41).

5.3 *Lie Algebraic Treatment of Space Charge*

Sections 5.2 and 5.3 described the application of Lie algebraic methods to single-particle transport and to multiparticle transport in the case for which interparticle (space-charge) interactions are neglected. This section describes a new Lie algebraic approach that, in certain circumstances, makes it possible to treat both linear and nonlinear space-charge effects in a rapid and precise way (42; for more detail, see 33). It should be of use in the design of accelerators and beam transport systems for which space-charge effects are important, but not completely dominant, and for which one is primarily interested in the behavior of the core of the charge distribution. In particular, using these methods it should be possible to construct accelerator and beam transport systems in such a way that linear and nonlinear space-charge effects are compensated by specially designed linear and nonlinear beam-line elements.

The Lie algebraic treatment of space charge begins with the Vlasov equation. [The Vlasov equation is a nonlinear partial differential equation that governs the evolution of particle density in phase space.] Suppose now that $h(z)$ is the distribution function describing the density of particles in phase space at some initial time. Suppose further that $g(z,t)$ is the dis-

tribution function describing the density of particles in phase space at general time t. That is, g is the solution of the Vlasov equation with the initial condition

$$g(z,0) = h(z). \tag{63.}$$

Then, in analogy to the previous discussion, it can be shown that there is a symplectic map $\mathcal{M}(t)$ such that

$$g(z,t) = h(\mathcal{M}^{-1}z). \tag{64.}$$

Consequently, the solution of the Vlasov equation is equivalent to the determination of a certain map $\mathcal{M}$.

Moreover, it can be shown that $\mathcal{M}$ obeys an equation of motion similar to Equation 44,

$$\dot{\mathcal{M}} = \mathcal{M}: -H[\mathcal{M}]:. \tag{65.}$$

However, in this case there is the added complication that the Hamiltonian is itself a functional of the map in question. That is, H depends on $g(z,t)$ because of space-charge forces, and $g(z,t)$ depends on $\mathcal{M}$. Physically, this complication arises because the phase-space distribution must evolve in a self-consistent manner.

Again, as in Section 3.5, it is possible to express $\mathcal{M}$ in factored product form; and again, as in Section 3.9, it is possible to derive equations of motion for the quantities R, f_3, f_4, etc. Naturally in this case the equations are much more complicated because they describe a self-consistent evolution. For example, in lowest approximation, it can be shown that R obeys a set of equations that can be roughly related to the Kapchinskij-Vladimirskij equations (33, 43).

Despite their far greater complexity, it is again possible to integrate these equations of motion numerically. When this is done, one obtains a self-consistent transfer map $\mathcal{M}$. As has been described, $\mathcal{M}$ can be used to obtain the complete phase-space density $g(z,t)$. Of course, $\mathcal{M}$ can also be used to find the trajectory of any individual particle in the distribution. In particular, $\mathcal{M}$ gives a complete description, including nonlinear aberration effects, of the optical properties of a system in the presence of space charge.

The procedure just outlined for the self-consistent calculation of transfer maps including space-charge effects has been realized in a substantial (although not yet fully complete) way in the computer program CHARLIE. CHARLIE takes as input the initial distribution function $h(z)$ as well as all information describing the beam-line elements of the beam transport or accelerator system to be studied, and provides $\mathcal{M}$ as output. As might be imagined, the construction of CHARLIE represents a major effort. In particular, CHARLIE contains all of GENMAP plus routines

for calculating $h(\mathcal{M}^{-1}z)$ to give the phase-space distribution, routines for various other Lie algebraic operations including map inversion, routines for computing charge and current densities from the phase-space distribution, and routines for solving the static Maxwell equations. CHARLIE currently works through third (octupole) order, and could in principle be extended to higher orders.

All tests to date indicate that CHARLIE gives results comparable to those produced by particle-in-cell (PIC) codes inregimes where both codes are expected to be applicable. However, CHARLIE runs approximately 300 times faster than PIC codes. Moreover, CHARLIE does not suffer from the statistical noise that makes it extremely difficult, if not impossible, to extract nonlinear aberration data from PIC code results. Thus, CHARLIE seems ideally suited for the study and compensation of both linear and nonlinear space-charge aberration effects.

6. ADVANCED APPLICATIONS

The purpose of this section is to describe briefly some of the applications of advanced Lie algebraic methods to the analysis of transfer maps and tracking data.

6.1 *Calculation of Closed Orbit*

Suppose $\mathcal{M}$ is the one-turn transfer map for a reentrant (circular) machine, and suppose $\mathcal{M}$ is factored in the form of Equation 31. Then, there exists a first-order polynomial g_1 such that $\mathcal{M}$ can be written in the form

$$\mathcal{M} = \exp(-:g_1:)\beta \exp(:g_1:), \tag{66a.}$$

where β has the form

$$\beta = \exp(:g_2:)\exp(:g_3:)\exp(:g_4:)\cdots. \tag{66b.}$$

In the language of Section 4.3, Equations 66 are an example of a conjugacy theorem. For a proof of Equations 66, see (26).

The map $\exp(:g_1:)$ may be viewed as the transformation that gives the coordinates of the closed orbit for the machine in terms of the coordinate system associated with what would have been the design orbit in the absence of errors. Thus, the calculation of g_1 is equivalent to finding the closed orbit. This calculation can be carried out for any given $\mathcal{M}$ by standard Lie algebraic techniques available in the codes MARYLIE 3.1 and MARYLIE 5.1. Consequently, it is possible to compute the closed orbit directly from the one-turn transfer map without the use of particle tracking.

Since $\exp(:g_1:)$ is the map going to closed orbit coordinates, it follows

that $\mathscr{M}$ is the one-turn map describing betatron motion about the closed orbit. Thus, all information about the behavior of orbits near the closed orbit is contained in $\mathscr{M}$. Note that $\mathscr{M}$ contains no first-order polynomials. Consequently, $\mathscr{M}$ maps the origin of phase space into itself as expected.

6.2 *Calculation of Chromaticity and Anharmonicity*

Suppose the one-turn map $\mathscr{M}$ of the previous section is a static map. That is, the polynomials $f_1, f_2, f_3, \ldots$ do not contain the time coordinate. (This will be the case if the machine contains no time-dependent elements such as rf cavities.) Then there is a static map $\mathscr{A}$ such that $\mathscr{M}$ can be written in the form

$$\mathscr{M} = \mathscr{A}^{-1}\mathscr{N}\mathscr{A}. \tag{67a}$$

Here $\mathscr{N}$ is a map in the normal form

$$\mathscr{N} = \exp(-:H:), \tag{67b}$$

with H being a polynomial with very special properties. Specifically, through terms of third order, H has the following special form:

$$H = (w_x + w_x' p_\tau + w_x'' p_\tau^2)h_x + (w_y + w_y' p_\tau + w_y'' p_\tau^2)h_y + ah_x^2 + bh_x h_y + ch_y^2 + dp_\tau^2 + ep_\tau^3 + fp_\tau^4. \tag{67c}$$

Here h_x and h_y are the quadratic polynomials

$$h_x = (x^2 + p_x^2)/2,$$
$$h_y = (y^2 + p_y^2)/2. \tag{67d}$$

The variable p_τ is related to energy deviations and is canonically conjugate to the variable τ describing time deviations. All other quantities appearing in H are constants. They have the following interpretation:

1. The constants w_x and w_y are phase advances giving the "tunes" $(= w/2\pi)$ of the on-energy closed orbit.
2. The constants w_x' and w_y' are first-order chromaticities that describe how tunes depend on energy deviations to first order.
3. The constants w_x'' and w_y'' are second-order chromaticities.
4. The constants a, b, and c are "anharmonicities" that describe how tunes depend on betatron amplitudes.
5. The constants d, e, and f are time-like drift terms, including nonlinear corrections, that describe how the time of flight depends on energy. See Section 3.4.

Observe that, because H depends only on h_x, h_y, and p_τ, the map $\mathscr{N} = \exp(-:H:)$ has the property that it sends circles in the x, p_x and y, p_y planes into themselves. Consequently, the map $\mathscr{N}$ describes idealized betatron motion.

The map $\mathscr{A}$ also has a physical interpretation. It can be shown that $\mathscr{A}$ gives complete information about all linear and nonlinear Twiss parameters and lattice functions including nonlinear distortion functions. Thus, one may say that the map $\mathscr{N}$ describes idealized betatron motion, and the maps $\mathscr{A}$ and $\mathscr{A}^{-1}$ describe the transformations between the actual betatron motion and the idealized betatron motion.

Equation 67 is again a Lie algebraic conjugacy theorem. Correspondingly, there are standard Lie algebraic tools in the various MARYLIE codes for the computation of $\mathscr{N}$ and $\mathscr{A}$ directly from the one-turn map. Equation 67 presents results through third order. The mathematical machinery now exists to compute chromaticities and anharmonicities through any order, and is implemented through fifth order in MARYLIE 5.1. The theory behind these calculations, and normal form methods in general, is not yet completely documented. What documentation exists can be found in (44–53).

6.3 *Calculation of KAM Tori and Analysis of Tracking Data*

We define a perfect torus to be the set of points in phase space that are the topological product of circles in the x, p_x and y, p_y planes in the static case, and the topological product of circles in the x, p_x and y, p_y and τ, p_τ planes in the dynamic case. Then it is obvious that $\mathscr{N}$ maps perfect tori into themselves in the static case, and it can be shown that the analog of $\mathscr{N}$ in the dynamic case also maps perfect tori into themselves.

Consider the action of the map $\mathscr{A}$. Since $\mathscr{A}$ is continuous and invertible, it must preserve topology. Consequently, the image of a perfect torus under the action of $\mathscr{A}$ must be a set of points that still has the topology of a torus. This set of points is called a distorted torus.

By construction, $\mathscr{A}$ maps perfect tori into distorted tori; and conversely, $\mathscr{A}^{-1}$ maps distorted tori into perfect tori. Also, as we have seen in the previous section, the maps $\mathscr{A}$ and $\mathscr{A}^{-1}$ describe the transformation between actual and idealized betatron motion. Finally, we have seen that $\mathscr{N}$ maps perfect tori into themselves. It follows that $\mathscr{M}$ maps distorted tori into themselves. Consequently, the distorted tori are Kolmogorov-Arnold-Moser (KAM) tori.

The existence of KAM tori is related to long-term stability. They are described, for example in (54). KAM tori for nonintegrable systems are isolated if they exist at all, and the demonstration of their existence is quite delicate. Correspondingly, normal form procedures are generally expected to be divergent when carried out to arbitrarily high order, and the dis-

cussion of this section and Section 6.4 generally has only asymptotic validity. The main use of normal form procedures in this context is to "remove" gross features of the motion so that the remaining features of the motion can be analyzed in greater detail.

The previous discussion can be used to good advantage by turning it around. Suppose a set of tracking data is produced by following various initial conditions through a large number of turns in a circular machine. How does one test to see if the points in the tracking data lie on various KAM tori? Simply transform the tracking data by applying the map $\mathscr{A}^{-1}$ to all the points in the tracking data. Then if the original points were on various KAM tori, the transformed points should be on perfect tori. Finally, the presence of perfect tori is easily detected simply by making two-dimensional projections into the q_i, p_i planes. The transformed data, when projected into these planes, should lie on perfect circles (45).

As an example of this procedure, look again at the Tevatron tracking data of Figure 3. From these data it is difficult to conclude anything about the presence of KAM tori. By contrast, Figure 4 shows the result of transforming the tracking data by $\mathscr{A}^{-1}$ using fifth-order MARYLIE. Evidently, despite the strong nonlinearities produced by the strongly powered Tevatron distortion sextupoles, the transformed points lie on nearly perfect circles. We conclude that to the order of the calculation, the original tracking data points lie on or very nearly on KAM tori.

The small residual scattering of points in the outer circles of Figure 4 may be the result of a need to go to even higher than fifth order. It may also be an indication of small-scale chaotic behavior, in which case there may only be the "remnants" of a KAM torus in this phase-space vicinity.

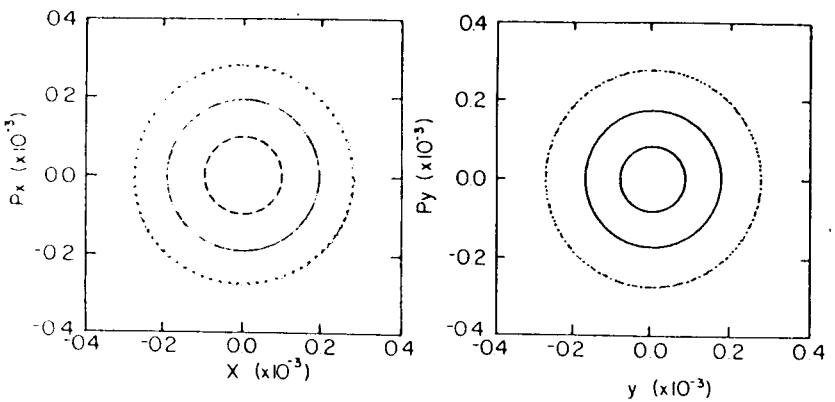


Figure 4 Turn-by-turn horizontal (*left*) and vertical (*right*) projections of the phase-space data of Figure 3 transformed by $\mathscr{A}^{-1}$ through fifth order.

It can be shown that these points are quite near the edge of the dynamic aperture, and thus it is quite remarkable that normal form procedures work as well as they do. See Section 6.5 for a description of the dynamic aperture.

6.4 *Calculation of Nonlinear Invariants and Linear Aperture*

Another way of saying that $\mathscr{N}$ maps perfect tori into themselves is to observe that $\mathscr{N}$ leaves invariant the functions h_x and h_y (and h_τ in the case of a dynamic map). That is, we have the relations

$$\mathscr{N}h_x = h_x, \text{ etc.} \tag{68.}$$

Since $\mathscr{N}$ is transformed into $\mathscr{M}$ under the action $\mathscr{A}$ and $\mathscr{A}^{-1}$, it follows that $\mathscr{M}$ has as invariants the functions I^x and I^y (and I^τ in the dynamic case) defined by the equations

$$I^x = \mathscr{A}^{-1}h_x, \text{ etc.} \tag{69.}$$

At this point it should be remarked that in writing the relations shown in Equations 68 and 69, it has been assumed that the action of a symplectic map on a function can be defined, whereas Section 2.2 only defined the action of a symplectic map on the phase-space variables. To obtain the action of a symplectic map on a function, note that Equation 18 defines the action of a Lie transformation on an arbitrary function g, and Sections 3.3 and 3.5 showed that any symplectic map can be written in terms of Lie transformations. Thus, the action of symplectic maps on functions is also well defined. In particular, one can show that if $\mathscr{M}$ is any symplectic map and g is any function, then one has the relation

$$\mathscr{M}g(z) = g(\mathscr{M}z). \tag{70.}$$

The ability to evaluate the action of a symplectic map on a function is a standard feature of the various MARYLIE codes. For a derivation of Equation 70, see (22).

To return to the main topic of this section, suppose the invariants I^x, etc are expanded in Taylor series in the form

$$I^x = I^x_2 + I^x_3 + I^x_4 + \ldots. \tag{71.}$$

Then it can be shown that the quadratic polynomials I^x_2, etc are the familiar Courant-Snyder "invariants." The Courant-Snyder invariants are single-particle quantities that are constant from turn to turn in the absence of nonlinearities (55). For a discussion of the Courant-Snyder invariants from a Lie algebraic perspective, see (22). Thus, the full invariants are nonlinear generalizations of the Courant-Snyder invariants. Moreover, the KAM

tori described in the previous section are simply those surfaces in phase space given by the relations I^x = constant, I^y = constant, etc.

It should be noted that the invariants described in this section are not to be confused with the moment invariants of Section 5.2. The moment invariants may be viewed as multiparticle "kinematic" invariants in that they involve a particle distribution and do not depend on the map (save that it is linear). By contrast, the invariants of this section are single-particle "dynamic" invariants and, according to Equation 69, depend on a^{-1}, which in turn depends on the map $\mathcal{M}$.

One of the criteria currently being explored for good accelerator design is that a machine should have a large "linear" aperture (56; see also 57, p. 129). The linear aperture is defined to be that region in phase space for which the value of the ordinary quadratic Courant-Snyder invariant exhibits only modest changes from turn to turn. We conclude from Equation 71 that for the linear aperture to be large, the higher order terms I_3^x, I_4^x, . . . , must be small.

From the previous discussion, it is evident that the nonlinear invariants in Equation 69 and their expansions in Equation 71 can be calculated directly from the one-turn map using Lie algebraic methods. Indeed, the various MARYLIE codes have standard options for carrying out such calculations for both static and dynamic maps. It follows that the linear aperture can be computed directly from the one-turn map without the need for particle tracking (49).

As an example of the behavior of the nonlinear invariants, Figures 5

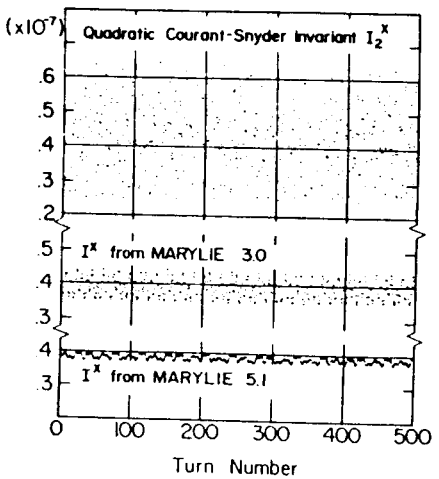


Figure 5 Turn-by-turn values of the horizontal invariant I^x computed through various orders. (See text for detailed discussion.)

and 6 show the turn-by-turn values of the series in Equation 71 computed through various orders for the case of the Tevatron with the distortion sextupoles powered. Figure 5 shows turn-by-turn values of $h_x(\mathcal{A}^{-1}z)$ evaluated for the phase-space data corresponding to the outer points in Figure 3. For the top set of points in Figure 5, only the linear portion of $\mathcal{A}^{-1}$ is retained, and the result is equivalent to evaluating the quadratic Courant-Snyder invariant. For the middle set of points, $\mathcal{A}^{-1}$ is truncated beyond third order, and $\mathcal{A}^{-1}$ through fifth order is used for the bottom set of points. Figure 6 shows the corresponding results for $h_y(\mathcal{A}^{-1}z)$.

Evidently, the quadratic Courant-Snyder terms alone show very large fluctuations due to the nonlinearities produced by these sextupoles. However, as successively more higher order terms are included, the full invariants become remarkably constant.

Similar calculations have been carried out for the two other set of phase-space data in Figure 3. In these cases, as might be expected since nonlinear effects are now less important, one finds that the full invariants are even more nearly constant.

6.5 *Other Applications*

The previous few sections have briefly described the application of advanced Lie algebraic methods to some selected problems. There are several other applications that are beyond the scope of this article. One such application is the design of third and higher order achromats (53). Roughly speaking, an achromat is a collection of elements that bends a

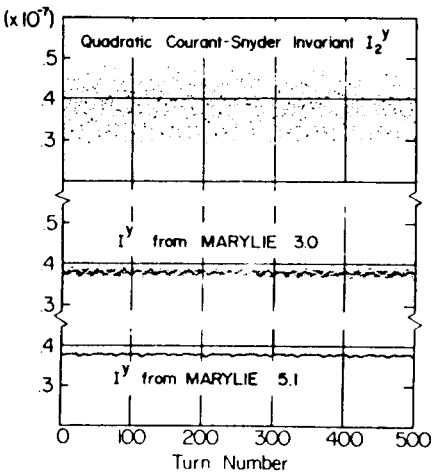


Figure 6 Turn-by-turn values of the vertical invariant I^y computed through various orders. (See text for detailed discussion.)

charged-particle beam but in all other respects, as far as possible, acts as the identity map.

Another application is the calculation of resonant normal forms and resonance widths. In the discussions of Sections 6.3 and 6.4, it was tacitly assumed that the phase advances (tunes) were away from certain resonant values. There are analogous Lie algebraic methods for the cases where phase advances are near resonant values. These methods make it possible to calculate the location of unstable periodic orbits and their associate separatrices, and to study the break up of KAM tori (41).

A major goal of such research is the calculation of the dynamic aperture of a circular machine directly from the one-turn map without the need for long-term tracking studies. (Roughly speaking, the dynamic aperture is that region in phase space for which trajectories exhibit long-term confinement, but not necessarily nearly linear motion.) It is evident that such information must be stored in the coefficients of the polynomials f_1, f_2, f_3, . . . in the factorization of Equation 31. If this information could eventually be extracted in a routine way, it would be much easier to explore the relative merits of various lattice designs and to minimize the effect of beam-element (magnet) imperfections on machine performance. With the advent of ever larger and more costly machines such as the proposed Superconducting Super Collider, the ability to predict accurately and to guarantee machine performance in advance is clearly a subject of major importance.

7. CONCLUDING DISCUSSION

A new procedure has been outlined for treating charged-particle optics. This procedure is computationally superior to earlier procedures and also provides both powerful new analytic tools and major new insight. In brief, the use of Lie algebraic methods provides an operator extension of the matrix methods of paraxial optics to the general case. These operators can be used to characterize and analyze departures from linear (paraxial) behavior, and to examine what can be done to control and compensate undesired effects. Thus, it should be possible eventually to analyze nonlinear behavior with the same facility that we now analyze linear behavior. It is expected that the use of Lie algebraic methods will lead to both improved understanding and improved design in many areas of charged-particle optics and accelerator physics.

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