Nonlinear Beam Dynamics Part 3: Lie Transformations

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In this lecture, we shall discuss methods for constructing transfer maps for accelerator elements. We have already seen how to do this for a drift space: but this is a special case, because the equations of motion can be solved exactly.

In this lecture, we shall discuss two powerful techniques for constructing (and representing) maps for accelerator elements:

• Lie transformations;

We shall use a sextupole as an example, but the techniques we develop are quite general.

Recall the general Hamiltonian for an accelerator element:

$$H = -(1+hx)\sqrt{\left(\frac{1}{\beta_0} + \delta - \frac{q\phi}{P_0c}\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2 \gamma_0^2}}$$
$$-(1+hx)a_s + \frac{\delta}{\beta_0}.$$
 (1)

For a drift space, this becomes:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2 \gamma_0^2} + \frac{\delta}{\beta_0}}.$$
 (2)

The equations of motion are given by Hamilton's equations:

$$\frac{dx}{ds} = \frac{\partial H}{\partial p_x}, \quad \frac{dp_x}{ds} = -\frac{\partial H}{\partial x},\tag{3}$$

and similarly for (y, p_y) and (z, δ) .

The equations of motion for a drift space are easy to solve, because the momenta p_x , p_y and δ are constants of the motion. The solution can be expressed as a map in closed form: the Hamiltonian is integrable.

For the transverse variables:

$$x_1 = x_0 + \frac{p_{x0}}{p_s} \Delta s, \qquad p_{x1} = p_{x0},$$
 (4)

$$y_1 = y_0 + \frac{p_{y0}}{p_s} \Delta s, \qquad p_{y1} = p_{y0}.$$
 (5)

And for the longitudinal variables, we have:

$$z_1 = z_0 + \left(\frac{1}{\beta_0} - \frac{\frac{1}{\beta_0} + \delta}{p_s}\right) \Delta s, \quad \delta_1 = \delta_0.$$
 (6)

The value of p_s (a constant of the motion) is given by:

$$p_s = \sqrt{\left(\frac{1}{\beta_0} + \delta_0\right)^2 - p_{x0}^2 - p_{y0}^2 - \frac{1}{\beta_0^2 \gamma_0^2}}.$$

A sextupole field can be derived from the vector potential:

$$A_x = 0, \quad A_y = 0, \quad A_s = -\frac{1}{6} \frac{P_0}{q} k_2 \left(x^3 - 3xy^2\right).$$
 (7)

This potential gives the fields:

$$B_x = \frac{P_0}{q} k_2 x y, \quad B_y = \frac{1}{2} \frac{P_0}{q} k_2 (x^2 - y^2), \quad B_s = 0.$$
 (8)

Note that the sextupole strength k_2 is given by:

$$k_2 = \frac{q}{P_0} \frac{\partial^2 B_y}{\partial x^2}. (9)$$

The normalized potential \vec{a} is given by:

$$\vec{a} = \frac{q}{P_0} \vec{A}. \tag{10}$$

Hence, the Hamiltonian for a sextupole can be written:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2 \gamma_0^2} + \frac{1}{6} k_2 \left(x^3 - 3xy^2\right) + \frac{\delta}{\beta_0}}.$$
(11)

Since the coordinates x and y appear explicitly in the Hamiltonian, the momenta p_x and p_y are not constants. The equations of motion are nonlinear, and rather complicated. We will not even bother to write them down, since we cannot find an exact solution in closed form: the Hamiltonian is not integrable.

To track a particle through a sextupole, we have to take one of two approaches:

- 1. integrate the equations of motion numerically (e.g. using a Runge–Kutta algorithm) with given initial conditions, or,
- 2. make some approximations that will enable us to write down an *approximate* map in closed form.

Lie transformations

Numerical techniques, such as Runge–Kutta algorithms, for integrating equations of motion are standard. The drawback in their use for accelerator beam dynamics is that they tend to be rather slow. Often, we are interested in tracking tens of thousands of particles, thousands of times around storage rings consisting of thousands of elements. Numerical integration is no good for this.

We shall therefore focus on the second approach. We shall make some approximations that will enable us to write down a map in closed form. There are various ways to do this: we begin by developing the idea of *Lie transformations*.

Lie transformations provide a means to construct a transfer map in closed form, even from a Hamiltonian that is not integrable. It is necessary to make some approximations, and these need to be understood in some detail. Suppose we have a function f of the phase space variables, coordinates \vec{q} and conjugate momenta \vec{p} :

$$f = f(\vec{q}, \vec{p}). \tag{12}$$

Suppose we evaluate f at the location in phase space for a particle whose dynamics are governed by a Hamiltonian H.

The time evolution of f is:

$$\frac{df}{dt} = \frac{d\vec{q}}{dt}\frac{\partial f}{\partial \vec{q}} + \frac{d\vec{p}}{dt}\frac{\partial f}{\partial \vec{p}}.$$
 (13)

Using Hamilton's equations, this becomes:

$$\frac{df}{dt} = \frac{\partial H}{\partial \vec{p}} \frac{\partial f}{\partial \vec{q}} - \frac{\partial H}{\partial \vec{q}} \frac{\partial f}{\partial \vec{p}}.$$
 (14)

We define the *Lie operator* :g: for any function $g(\vec{q}, \vec{p})$:

$$g: = \frac{\partial g}{\partial \vec{q}} \frac{\partial}{\partial \vec{p}} - \frac{\partial g}{\partial \vec{p}} \frac{\partial}{\partial \vec{q}}.$$
 (15)

Constructing a Lie operator from the Hamiltonian, we can write:

$$\frac{df}{dt} = -:H:f. \tag{16}$$

Equation (16) suggests that given f at time $t = t_0$, we can evaluate f at any later time $t_0 + \Delta t$:

$$f(t_0 + \Delta t) = e^{-\Delta t : H:} f\Big|_{t=t_0}.$$
 (17)

Here, the exponential of the Lie operator is defined in terms of a series expansion:

$$e^{-\Delta t : H:} = 1 - \Delta t : H: + \frac{\Delta t^2}{2} : H:^2 - \frac{\Delta t^3}{3!} : H:^3 + \cdots$$
 (18)

Equation (16) does indeed give us the value of f at any time $t_0 + \Delta t$, given the value of f at $t = t_0$.

We can see this by simply making a Taylor series expansion:

$$f(t_0 + \Delta t) = f(t_0) + \Delta t \frac{df}{dt} \Big|_{t=t_0} + \frac{\Delta t^2}{2} \frac{d^2 f}{dt^2} \Big|_{t=t_0} + \frac{\Delta t^3}{3!} \frac{d^3 f}{dt^3} \Big|_{t=t_0} + \cdots$$
(19)

Then, since from (16) we can write:

$$\frac{d}{dt} = -:H: \tag{20}$$

equation (18) follows.

The operator $e^{g:}$ is called a *Lie transformation*.

To see how to use Lie transformations to solve the equations of motion for a given system, consider a familiar example: a simple harmonic oscillator in one degree of freedom.

The Hamiltonian is:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2. \tag{21}$$

Suppose we want to find the coordinate q as a function of time t. Of course, in this case, we could simply write down the equations of motion (from Hamilton's equations) and solve them (because the Hamiltonian is integrable). However, we can also write:

$$q(t_0 + \Delta t) = e^{-\Delta t : H:} q \Big|_{t=t_0}.$$
 (22)

To evaluate the Lie transformation, we need :H:q. This is given by (15):

$$:H:q = \frac{\partial H}{\partial q} \frac{\partial q}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial q}{\partial q} = -\frac{\partial H}{\partial p} = -p. \tag{23}$$

Similarly, we find:

$$:H:p = \omega^2 q. \tag{24}$$

This means that:

$$:H:^{2}q = :H:(-p) = -\omega^{2}q, \tag{25}$$

$$:H:^{3}q = :H:(-q) = \omega^{2}p, \tag{26}$$

and so on.

Using the above results, we find:

$$q(t_0 + \Delta t) = q|_{t=t_0} - \Delta t : H : q|_{t=t_0} + \frac{\Delta t^2}{2} : H :^2 q|_{t=t_0} - \cdots$$
(27)

$$= q(t_0) + \Delta t \, p(t_0) - \omega^2 \frac{\Delta t^2}{2} q(t_0) - \cdots$$
 (28)

Collecting together even and odd powers of t, we find that equation (28) can be written:

$$q(t_0 + \Delta t) = q(t_0)\cos(\omega \Delta t) + \frac{p(t_0)}{\omega}\sin(\omega \Delta t). \tag{29}$$

Similarly (an exercise for the student!) we find that:

$$p(t_0 + \Delta t) = e^{-\Delta t : H:} p(t_0) \Big|_{t=t_0} = -\omega q(t_0) \sin(\omega \Delta t) + p(t_0) \cos(\omega \Delta t).$$
(30)

Equations (29) and (30) are the solutions we would have found using the conventional approach of integrating the equations of motion: but note that we have not performed any integrations, only differentiations (though we have had to sum an infinite series...)

Lie operators and Lie transformations have many interesting properties that makes them useful for analysing the behaviour of dynamical systems. We shall explore these properties further in the next lecture; but for now, we shall simply see how to apply the technique demonstrated for the harmonic oscillator, to a particle moving through a sextupole.

Recall the Hamiltonian for a sextupole (11):

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2 \gamma_0^2}} + \frac{1}{6} k_2 \left(x^3 - 3xy^2\right) + \frac{\delta}{\beta_0}.$$

Using Lie operator notation, we can write the map for a particle moving through the sextupole as:

$$\vec{x}(s_0 + \Delta s) = e^{-\Delta s : H:} \vec{x}\Big|_{s=s_0}.$$
 (31)

Since the Lie transformation evolves the dynamical variables according to Hamilton's equations (for the Hamiltonian H) the map expressed in the form (31) is necessarily symplectic. Since application of a Lie transformation just involves differentiation and summation (of an infinite series) we can, in principle, apply the map in this form, for any Hamiltonian.

However, a map expressed as a Lie transformation is not explicit: it requires algebraic manipulation before we can simply put in the values of the dynamical variables at the entrance of the magnet, and obtain the values at the exit of the magnet.

For tracking simulations, it is much more useful to have an explicit map, which we can apply by simply substituting numbers into a given formula. For example, equations (29) and (30) give an explicit map for the harmonic oscillator.

To produce an explicit map, we can simply evaluate the Lie transformation for each of the dynamical variables, keeping terms in the series expansion up to some order in s.

To see how this works, let us apply the technique to a sextupole.

First of all, dealing with the full Hamiltonian for the sextupole makes things unnecessarily complicated. Let us assume that $\delta=0$, and that $y=p_y=0$. Then, we have motion in only one degree of freedom (x). Further, let us take the limit $\beta_0 \to 1$. Then, the Hamiltonian (11) becomes:

$$H = -\sqrt{1 - p_x^2} + \frac{1}{6}k_2x^3.$$

Now let us evaluate the Lie transformations of x and p_x . To first order in Δs , we find:

$$x(s_0 + \Delta s) = e^{-\Delta s : H:} x \Big|_{s=s_0} = x_0 + \frac{p_{x_0} \Delta s}{\sqrt{1 - p_{x_0}^2}} + O(\Delta s^2),$$
(32)

$$p_x(s_0 + \Delta s) = e^{-\Delta s : H:} p_x \Big|_{s=s_0} = p_{x_0} - \frac{1}{2} k_2 x_0^2 \Delta s + O(\Delta s^2).$$
 (33)

where $x_0 = x(s_0)$, etc.

If we truncate the sextupole map (32) and (33) to first order in Δs , we obtain:

$$x(s_0 + \Delta s) = x_0 + \frac{p_{x_0} \Delta s}{\sqrt{1 - p_{x_0}^2}},$$

$$p_x(s_0 + \Delta s) = p_{x0} - \frac{1}{2}k_2x_0^2\Delta s.$$

This map looks like the map for a drift space of length Δs , but with the addition of a momentum "kick" of size $-\frac{1}{2}k_2x_0^2\Delta s$. Note that the deflection is proportional to the square of the initial co-ordinate: this reflects the nonlinear nature of the field.

It is possible to use the above map for a sextupole in a tracking code. But we can expect to have lost a lot of accuracy by truncating the series expansion for the Lie transformation at first order in Δs . In fact, the truncation has a rather unpleasant consequence...

If we calculate the Jacobian J of the truncated map, and check for symplecticity, we find:

$$J^{\mathsf{T}}SJ = \begin{pmatrix} 0 & 1+\Delta \\ -1-\Delta & 0 \end{pmatrix} \tag{34}$$

where

$$\Delta = \frac{k_2 x_0 \Delta s^2}{\left(1 - p_{x0}^2\right)^{\frac{3}{2}}}.$$
 (35)

There is a "symplectic error" of order Δs^2 . If we require symplectic maps (for a tracking code, for example), this is bad news. However, we know that the full map, including all terms in the Lie transformation, must be symplectic. This implies that, if we keep more terms, the symplectic error must appear in higher order in Δs .

To reduce the "symplectic error" we can construct the map to second order in s. The result is:

$$x(s_0 + \Delta s) = x_0 + \frac{p_{x0}\Delta s}{\sqrt{1 - p_{x0}^2}} - \frac{k_2 x_0^2 \Delta s^2}{4\left(1 - p_{x0}^2\right)^{\frac{3}{2}}} + O(\Delta s^3),$$
(36)

$$p_x(s_0 + \Delta s) = p_{x0} - \frac{1}{2}k_2x_0^2\Delta s - \frac{k_2x_0p_{x0}\Delta s^2}{2\sqrt{1 - p_{x0}^2}} + O(\Delta s^3).$$
(37)

The higher order terms get increasingly complicated and difficult to interpret. It also very quickly gets cumbersome to work out the symplectic error — but we find, as expected, that if we work out the map to order N, then the symplectic error is of order N+1.

Summary

• The transfer map for an accelerator element can be represented in symplectic form as a Lie transformation:

$$\vec{x}(s) = e^{-Hs} \vec{x}(0),$$

where H is the Hamiltonian.

- An explicit map in the form of a power series can be obtained from a Lie transformation, by performing the appropriate differentiations. In general, a map in the form of an infinite series is produced.
- A map in a convenient form for tracking can be obtained by truncating the infinite series obtained by evaluating a Lie transformation. However, it may be necessary to retain high order terms in order to maintain accuracy, and reduce effects arising from the fact that the truncated map is no longer symplectic.